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# A HYBRID RANGING SYSTEM FOR SPACECRAFT

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## A HYBRID RANGING SYSTEM FOR SPACECRAFT

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### ABSTRACT

This report describes, in engineering terms, the principles and practice of satellite ranging by direct measurement of the elapsed time for a hybrid combination of sidetone-modulated and pseudo random noise-modulated, CW, RF energy to travel from the ground, to a spacecraft and back, after being transponded in a phase coherent manner at the spacecraft. A ranging subsystem utilizing sidetone-PN techniques was successfully built at the Goddard Space Flight Center and is now ready for final loop tests and integration into the GSFC Range and Range Rate System, to give the latter universal cisplanet ranging capabilities.

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The Hybrid Ranging System functions as follows: a demand pulse synchronized to WWV stores a binary pattern composed of transmitted bits and starts a time interval counter which is readied for stoppage when the identical signal is received. Simultaneously, sidetones, harmonically related to one another, are transmitted in alternately reversed

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phases, received in reversed phases and are used for vernier stop-control of the time interval counter. Thus, the non-ambiguous advantages of PN encoding are exploited without the cost of the wide bandwidth required for precise PN-only range measurements; and the precision and narrow bandwidth advantages of sidetone ranging are exploited without the cost of the engineering problems associated with ambiguity resolution by fractional cycle per second sidetones.

*Author*

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## A HYBRID RANGING SYSTEM FOR SPACECRAFT

### 1. Introduction

A spacecraft ranging system which utilizes both sidetone and encoded signals has been built in the Goddard Space Flight Center laboratories and has worked as a subsystem—it is now ready for final loop tests. This universal hybrid system capitalizes upon both the advantages of sidetone ranging which permits fine distance definition under restricted bandwidth conditions, and upon the advantages of pseudo random encoding which permits unambiguous ranging without the need for many low frequency sidetones and their associated problems. The new system eliminates the basic disadvantages of previous ranging systems: the unnecessarily wide bandwidths and complex coding techniques of the encoded-signal-only system; and the fractional cycle per second problems of the sidetone-only system at cisplanetary distances.

The hybrid system will be exploited to enhance the highly successful GSFC sidetone ranging system which has functioned with precision on Syncom in a special tracking network and which has made accurate range measurements on IMP in the general tracking network. With this modification, the GSFC Range and Range Rate System will have a universal ranging capability applicable to cislunar tracking problems such

as Apollo and cisplanet tracking problems such as non-ambiguous, apogee-ranging on projected IMP missions.

The purpose of this report is to present an overall, but brief description of the Hybrid ranging system. The Hybrid modification is compatible with the highly successful Goddard Space Flight Center's Range and Range Rate System, and augments its capabilities. In this modification of the sidetone system, known encoded ranging techniques are combined with direct RF transit time measurement and sidetone techniques to create a more optimum design than previously known designs.\* To distinguish the new system it is called the Hybrid System; it utilizes a "TIMER" coding technique (from: Time Interval Measurements with an Encoded Ranging System); it relies primarily upon direct measurement of the time required for both sidetones and an encoded, CW, RF signal to travel from the ground to the spacecraft and back, after being transponded in a phase coherent manner at the spacecraft. In this report the TIMER techniques are emphasized because they are new; but the significant advantages and the successful field performances of the precise sidetone ranging system are the base upon which the Hybrid ranging system is built.

This report is divided into five sections as follows:

Basic TIMER System, Some Properties of Maximal Linear Codes, Some

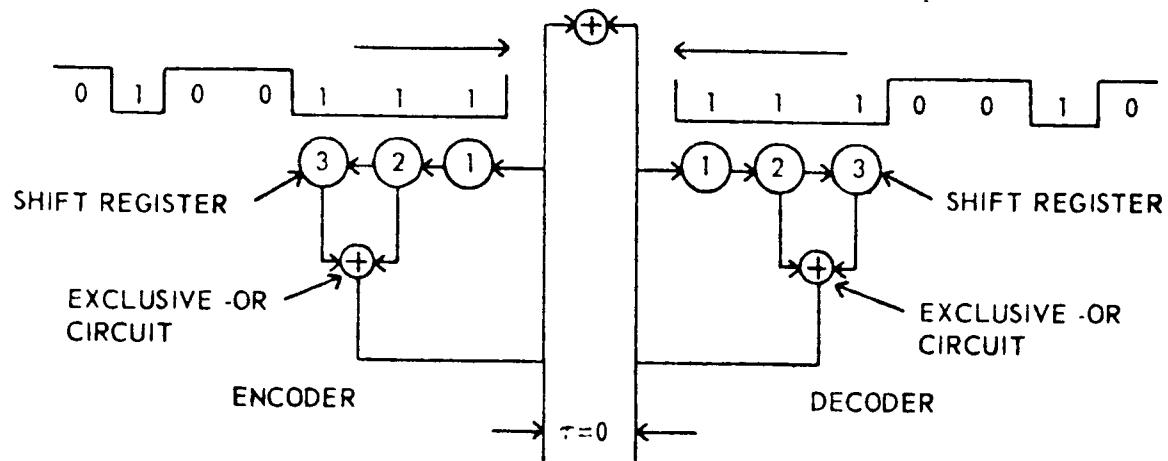
\*A number of the coding techniques described in this report were created by members of the Jet Propulsion Research Laboratory and were derived here from information contained in JPL Research Summary Reports 36-1, 36-2, 36-3 . . . etc. issued quarterly starting in 1960. Additional coding concepts were derived from other reports listed in the Bibliography.

**Properties of Acquirable Codes, Overall Description, and Hybrid System.** An Appendix describes the practical digital circuitry used to demonstrate the feasibility of the Hybrid version of the TIMER System. More expanded and detailed descriptions of individual circuits, codes, and, specifically, the Goddard Space Flight Center's Range and Range Rate System are contained in the reports listed in the Bibliography.

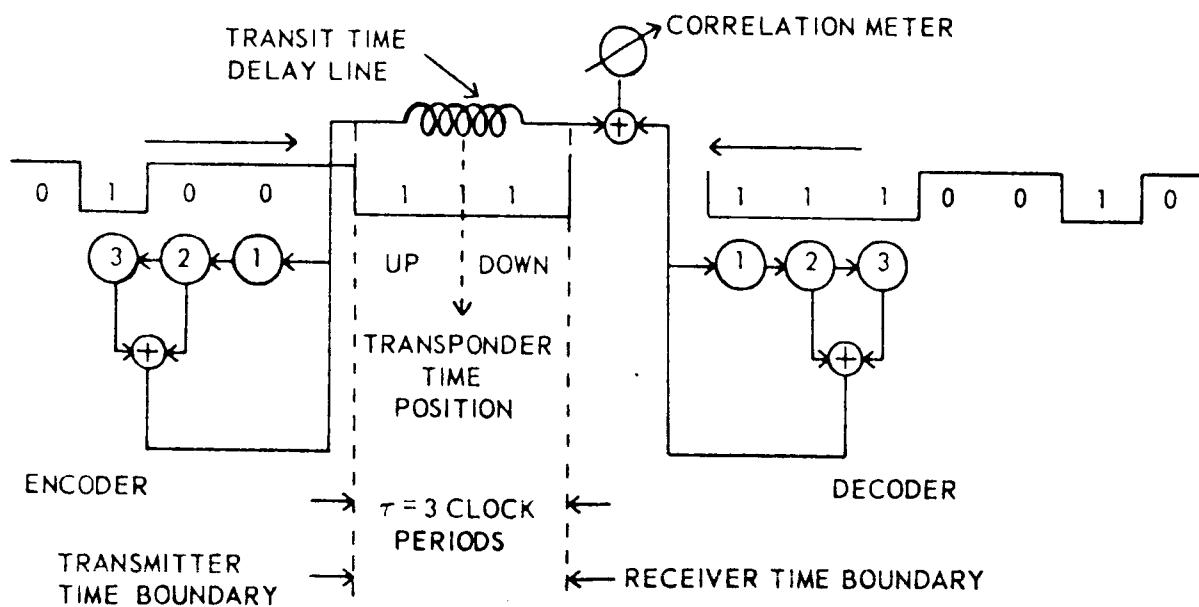
## 2. Basic TIMER System

Basically, the TIMER System determines the time delay between the transmission and reception of an unambiguous PN-encoded pattern. This technique which is closely related to simple pulse radar methods, requires no complex computer operations. The principles of range measurements made with this system are illustrated in the simplified block diagram shown in Figure 1.

A simple maximal linear code, 1 1 1 0 0 1 0, is used as an example only. If this code is continuously transmitted as 1 1 1 0 0 1 0 1 1 1 0 0 1 0 1 1 . . . etc., it can be broken up into seven unambiguous, sequential three-bit groups of 1 1 1, 1 1 0, 1 0 0, 0 0 1, 0 1 0, 1 0 1, and 0 1 1. Each sequential group of three bits is unambiguous and definitive in the sense that within the total code each three-bit word or pattern occurs only once; each word is unique. Thus, if a transmitted pattern composed of three bits is stored and compared to the delayed, received pattern, received within the time interval of the whole code, only one pattern out of those received will identically match the transmitted pattern.



A. ZERO DISTANCE CASE



B. TRANSIT TIME DELAYED CASE

Figure 1.

The encoder which modulates the transmitter, and the decoder which is "pattern-matched" to the received code, are each composed of a three-stage shift register with appropriate feed-back. The contents of the shift register flip-flops correspond during each bit-time interval to one of the three-bit patterns described above, and determine unambiguously the particular bit in the long code that is being transmitted or received as the case may be. Thus, if transit time,  $\tau$ , is zero (the encode and decode generators are synchronized and their outputs are compared with no time delay) then the instantaneous patterns in both generators are identical (Figure 1A). As the two generators are separated by a distance corresponding to a transit time of  $\tau = K$  (a constant), and the decode generator is kept locked to each received bit, the contents of the decode generator at time  $\tau$  correspond to the contents of the encode generator at time zero (Figure 1B).

If, on the other hand, the receiver space boundary moves towards (or away from) the transmitter boundary (equivalent to a continuous change in transit time) to simulate transponder velocity, and at the same time the decode generator creates bits at a faster (slower) rate to keep up with the faster (slower) rate at which bits are received, the previous arguments still hold. Thus, when the leading edge of a particular transmitted bit reaches the receiver time boundary, it is met, so to speak, by the corresponding bit from the decode generator—and the contents of the decode generator at time  $\tau$  will match the previous contents of the encode generator at time zero. In brief, the measurement of  $\tau$  by

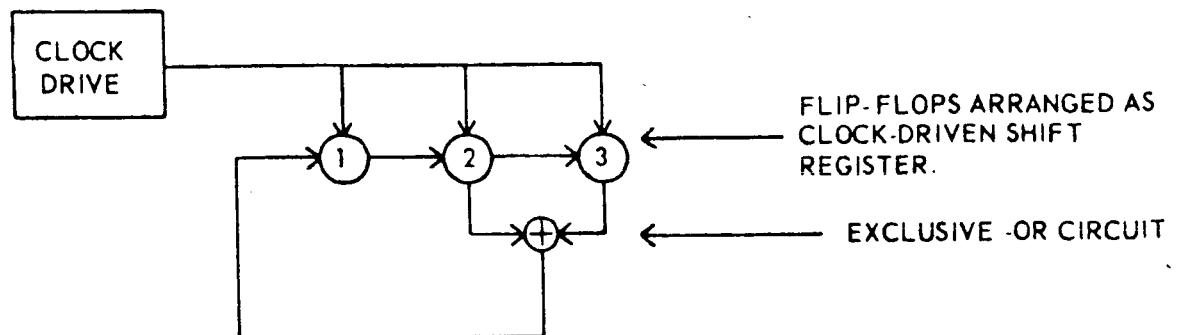
determining the elapsed time between the formation of an encode pattern and the formation of an equivalent decode pattern, is closely related to simple pulse radar techniques, and is in essence independent of Doppler effects. In addition, the present techniques are compatible with long time constant, narrow bandwidth, phase-locked loop acquisition techniques with their improved signal-to-noise properties.

In the following sections, the simplified example of the encoder given above is expanded into a more practical encoder suitable for lunar and cisplanet range measurements.

### 3. Some Properties of Maximal Linear Codes

Some of the pseudo random noise (PN) properties that are exploited in the TIMER System are illustrated below. As shown in Figure 2A, if three flip-flops are connected as a shift register, and the outputs of the last two stages are combined in a circuit, designated  $\oplus$  or exclusive-or circuit,\* which feeds a one back to the input whenever the last two stages are in different states, a code is generated which has almost ideal correlation properties. The states of the several flip-flops are tabulated in the table given in Figure 2B, and the generated code corresponds to the contents of the third flip-flop as indicated in the table. This code is called a maximal linear binary code or m-sequence (see Bibliography).

\*The exclusive-or function,  $F = A \cdot \bar{B} + B \cdot \bar{A}$ , is variously indicated in the technical literature as, exclusive-or,  $\oplus$ , mod-2 addition, modulo-2 addition, addition without carry and as a function which is true when two binary outputs disagree, and false when two binary outputs agree.



A. Three-Stage PN Generator

Time	State of Flip-Flops			Input to First Stage on Next Shift
	(1)	(2)	(3)	
$t_0$	1	1	1	0
$t_1$	0	1	1	0
$t_2$	0	0	1	1
$t_3$	1	0	0	0
$t_4$	0	1	0	1
$t_5$	1	0	1	1
$t_6$	1	1	0	1
$t_7$	1	1	1	0

B. Tabulation of Sequential States of Three Stage PN Generator

Figure 2

The output code is 1 1 1 0 0 1 0 and is repeated indefinitely as  
 1 1 1 0 0 1 0 1 1 1 0 0 ..... The length of the code, L, is  $2^n - 1$   
 where n is the number of flip-flops (i.e. the number of stages in the  
 shift register). If this code is shifted and added to the unshifted code,  
 according to the rule that a one is generated wherever an element of the  
 original and an element of the shifted identical code are different (ex-  
 clusive-or or mod-2 addition), the result will always be the same code  
shifted again as shown below (except when the code is shifted zero, or  
 a multiple of L bits):

original code	1 1 1 0 0 1 0 1 1 1 0 0 1 0 .....
---------------	-----------------------------------

code shifted by one bit	* 1 1 1 0 0 1 0 1 1 1 0 0 1 .....
-------------------------	-----------------------------------

resultant code	0 0 1 0 1 1 1 0 0 1 0 1 1 .....
----------------	---------------------------------

original code	1 1 1 0 0 1 0 1 1 1 0 0 1 0 .....
---------------	-----------------------------------

code shifted by two bits	* 1 1 1 0 0 1 0 1 1 1 0 0 .....
--------------------------	---------------------------------

resultant code	0 1 1 1 0 0 1 0 1 1 1 0 .....
----------------	-------------------------------

"	"	"
---	---	---

"	"	"
---	---	---

"	"	"
---	---	---

"	"	"
---	---	---

original code	1 1 1 0 0 1 0 1 1 1 0 0 1 0 1 ...
---------------	-----------------------------------

code shifted by five bits	* 1 1 1 0 0 1 0 1 1 1 1 1 ...
---------------------------	-------------------------------

resultant code	0 1 0 1 1 1 0 0 1 0 ...
----------------	-------------------------

Thus, these PN codes, have the highly important property that when  
 shifted and compared, mod-2 with the original code, the same code is

generated. And the resultant code has the same distribution of 1's and 0's as the original code which always has one more 1 than 0. It is noted here that the resultant code has four 1's and three 0's, and that a 1 indicates a disagreement, and a 0 indicates an agreement between the original and the shifted codes.

When the above-noted shift and add properties of the PN code are related to the simple binary correlation function described below, the nearly perfect correlation properties of PN codes become apparent. Binary correlation can be defined as follows:

$$\text{correlation} = \frac{\text{no. of agreements} - \text{no. of disagreements}}{\text{no. of agreements} + \text{no. of disagreements}}$$

or  $C = \frac{A - D}{A + D}$

Where C is the correlation factor, A the number of agreements, and D the number of disagreements. Inserting the numbers illustrated:

$$C = \frac{3 - 4}{3 + 4} = -\frac{1}{7} = -\frac{1}{L}$$

The correlation factor for 1 to L-1 shifts is always:

$$C = -\frac{1}{L} = \frac{-1}{2^n - 1}$$

because, for these codes, in general,

$$C = \frac{\frac{L-1}{2} - \frac{L+1}{2}}{L} = -\frac{1}{L}$$

In words, this is true because the exclusive -or, or mod-2 acquired code always contains one more disagreement than agreement; the acquired code is the original, but shifted, maximal linear pseudo random code.

Whenever the code is unshifted (or shifted a multiple of L bits) and added mod-2 to the original code (disagreements are 1's and agreements are 0's), all corresponding elements of the two codes agree,  $A = L$ ,  $D = 0$ , and

$$C = \frac{A - D}{A + D} = \frac{L - 0}{L + 0} = 1$$

In short mathematical form, the correlation factor derived by the processes illustrated above and the conclusions reached, can be described, for PN codes, as:

$$\begin{aligned} C(k) &= \frac{1}{L} \sum_{n=0}^{n=L-1-k} a_n \oplus a_{n-k} \\ &= -\frac{1}{L} \text{ for } k = 1 \text{ to } L - 1 \\ &= 1 \text{ for } k = 0 \text{ or } mL \end{aligned}$$

Where  $a_n$  is an element of the original code

$a_{n-k}$  is an element of the shifted code

$m$  is an integer

$k$  is an integer corresponding to the number of shifts of the shifted code.

$n$  is an integer.

To summarize, the correlation property of the PN code is essentially (for longer codes) zero when not matched exactly and unity when matched exactly. The PN codes possess nearly perfect correlation properties.

In the TIMER System, the local decoder code is "locked on" to the received code by automatic circuitry which measures the correlation

factor of the decoder code with the received code; the decoder code is driven by the received clock plus Doppler and shifted periodically by extra shifts until correlation is obtained. Long time constant integration and corresponding narrow bandwidth circuits enhance the signal to noise properties of this acquisition process.

Although a three flip-flop generator was selected as an example, codes of this type can be simply made for lengths up to  $2^{34}-1$  (about  $10^{10}$ ) and longer. It is not always true that the mod-2 or exclusive-or circuit is connected to the last two stages; other connections, as described below and in the reports listed in the Bibliography, are necessary for certain lengths.

In Table 1, some of the simpler connections for m-sequences are listed.

TABLE 1  
LINEAR MAXIMAL GENERATORS  
WITH SIMPLE CONNECTIONS\*

n	Stages Tapped	n	Stages Tapped
2	2, 1	18	18, 11
3	3, 2	20	20, 17
4	4, 3	21	21, 19
5	5, 3	22	22, 21
6	6, 5	23	23, 18
7	7, 5	25	25, 22
9	9, 5	28	28, 25
10	10, 7	29	29, 27
11	11, 9	31	31, 28
15	15, 14	33	33, 20
17	17, 14		

\*See Bibliography, Peterson, Appendix C.

#### 4. Some Properties of Acquirable Codes

To handle longer codes practically, they are broken up into shorter "acquirable" codes. These longer codes, composed of the shorter codes, can be relatively easily generated as illustrated in Figure 3. The generated code,  $W_n$ , is equal to  $x \oplus y z$  - it is the mod-2 sum of the  $x$  code with the  $y$  "logical and"  $z$  codes.

For the example illustrated in Figure 3, the overall code length  $L$ , is the product of the shorter codes  $L_x L_y L_z$ , or  $(2^3 - 1) (2^4 - 1) (2^5 - 1) = 3255$  bits. To acquire such a code, the shorter codes are "locked on"

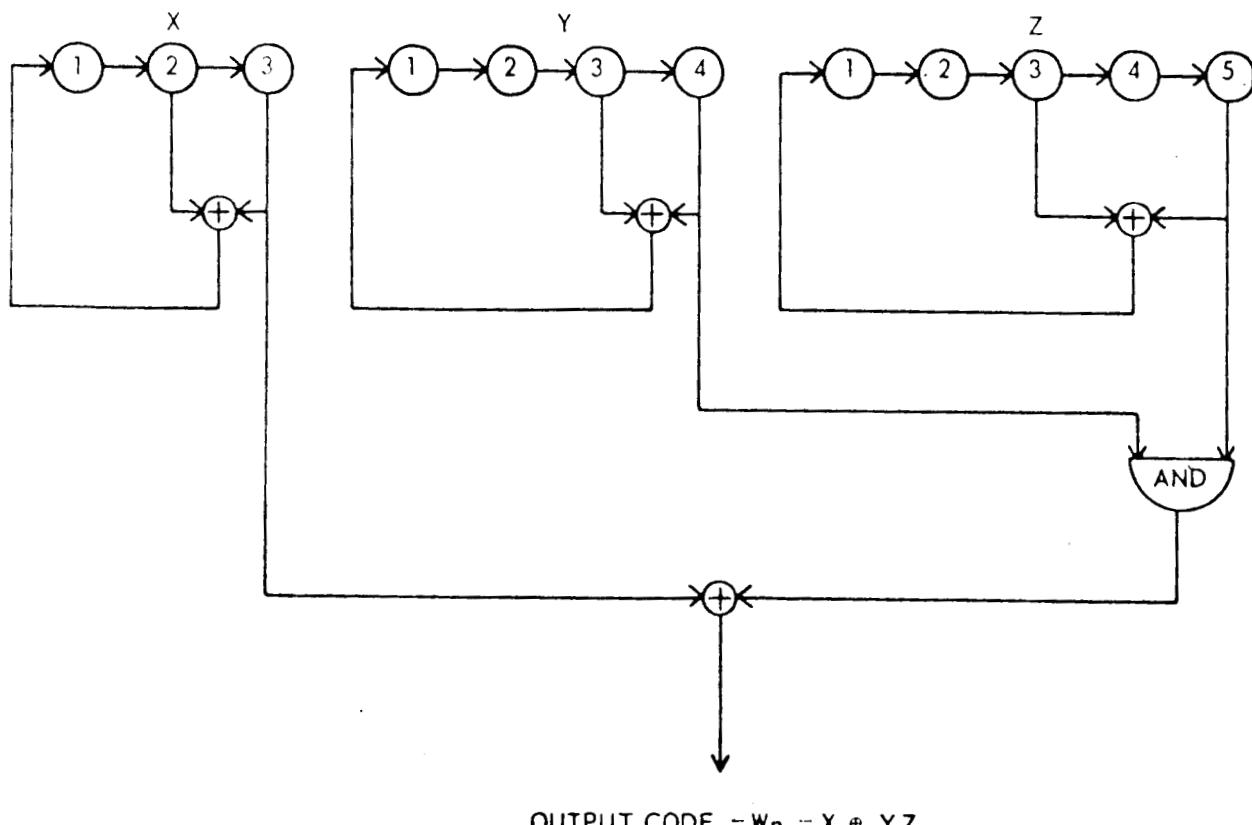


Figure 3. Acquirable Code Generator

to the total received code,  $W_R$ , usually sequentially, and the maximum number of shifts necessary to acquire the long code is  $Lx + Ly + Lz$  or  $7 + 15 + 31 = 53$  shifts - the  $x_m$  code is correlated with  $W_R$  first, then the  $x_m \oplus y_m$  combined codes, and finally the  $x_m \oplus z_m$  codes; after this process  $W_m$  the complete decoder code,  $(x_m \oplus y_m \oplus z_m)$  is completely "matched" or correlated with the received code,  $W_R$ .

The almost ideal correlation levels of  $-\frac{1}{L}$  and 1 for single-code to single-code correlation, are reduced to approximately  $-\frac{1}{L}$  and  $\frac{1}{2}$  for the "acquirable-code" correlation processes described above. As shown below, the "acquirable-code" acquisition process results in a change from a sequence of approximately random 1's and 0's (which exhibit nearly zero correlation) to a sequence of 1's and 0's of approximately  $\frac{1}{4}$  ones and  $\frac{3}{4}$  zeros (which exhibit nearly  $\frac{1}{2}$  correlation), when a given short code is correlated with the longer code. For example,

$$W \oplus x = x \oplus yz \oplus x = yz$$

and the probability code  $y$  and code  $z$  have the value of 1 at any time is approximately  $1/2$  times  $1/2$  or  $1/4$ . Thus

$$C = \frac{A - D}{A + D} = \frac{3/4 - 1/4}{1} = \frac{1}{2}$$

Also, if the  $x$  and  $y$  codes are correlated,

$$\begin{aligned} W \oplus x \oplus y &= x \oplus yz \oplus x \oplus y \\ &= y \oplus yz \\ &= y \cdot \overline{yz} + \bar{y} \cdot yz \quad (\text{by expansion}) \\ &= y \cdot (\bar{y} + \bar{z}) = y \cdot \bar{z} \quad (\text{by DeMorgan's theorem}) \end{aligned}$$

and again the probability that  $y$  "logical and"  $z$  have the value of 1 at any time is approximately  $1/4$  as above.

In the TIMER System, negative logic and -6 volts levels for true statements are used. As shown later, -3 volts indicate zero correlation, and -1.5 volts indicates 50% correlation. Automatic shifting and recognition circuitry acquire and lock the decoder codes with the received code, by measuring the change in voltage level from -3v to -1.5 volts. When all codes are acquired, the correlation indicator goes to 0 volts, i.e. 100% correlation.

## 5. Overall Description

By a simple extension of the principles described in the section called the Basic TIMER System, the advantages of acquirable codes can be exploited in the TIMER System as illustrated in Figure 4. Just as each one of the seven possible three bit words in the three flip-flop PN generator determines the bit being transmitted, so each of the four bit words and five bit words respectively for the four and five bit flip-flop PN generators are definitive. And the summation 12 bit word, composed of the 3, 4, and 5 bit words, defines exactly the particular bit of the 3255 bit code that is being transmitted. A timer can be initiated at the instant in time that a particular 12 bit pattern in the encoder generators is formed, and this pattern can be stored in a register; the timer can be stopped at the instant in time that the decoder generators, previously locked to the received code, match the stored encoder pattern. The timer, then, will indicate the transit time.

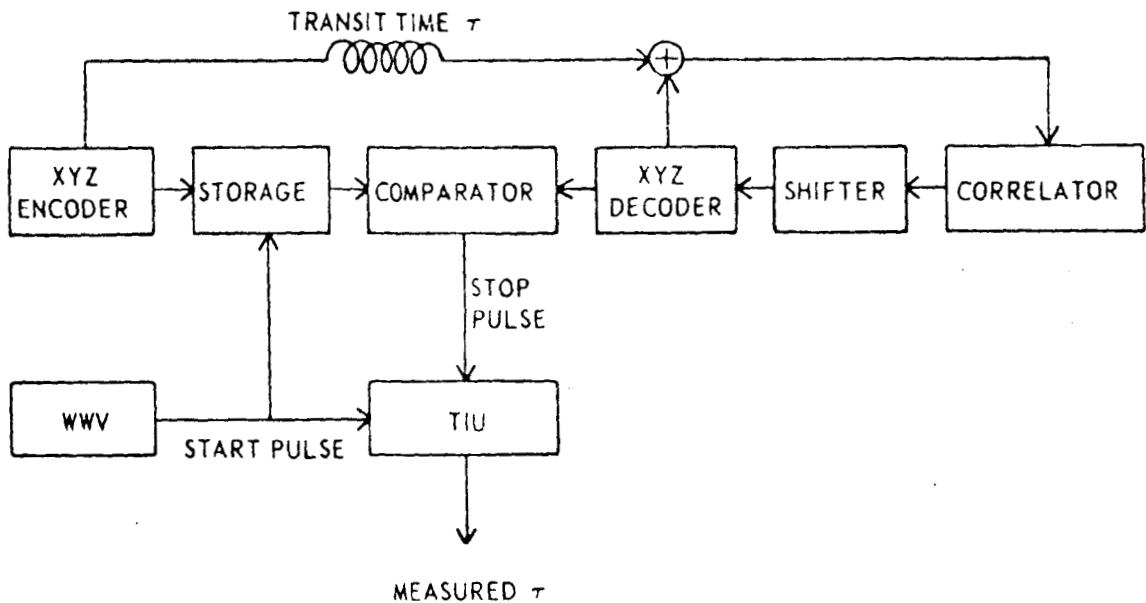
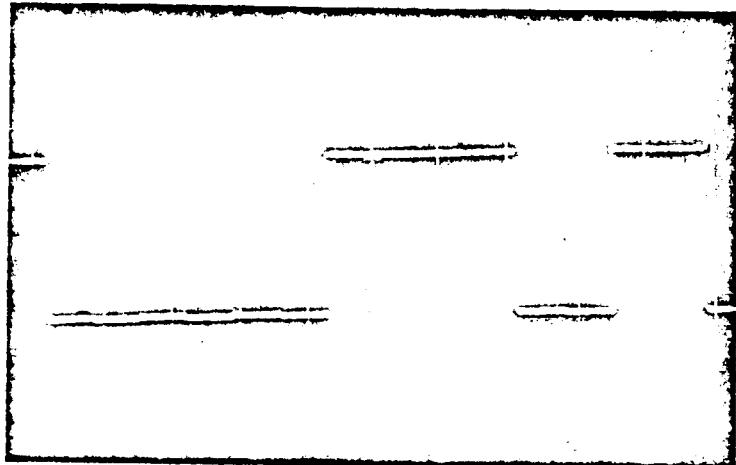
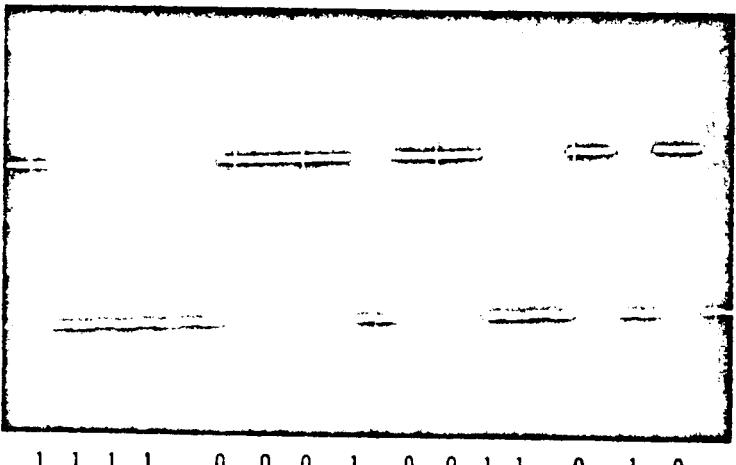


Figure 4.

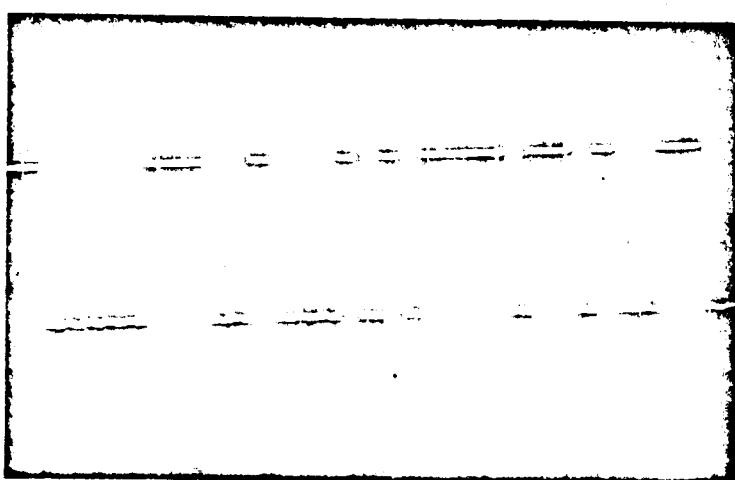
The timing actions that take place are the following: a demand pulse synchronized for timing purposes to WWV, stores the existing 3 bits of the  $X_n$  code, 1 1 1 0 0 1 0, in a storage register; simultaneously the existing 4 bits of the  $y_n$  code 1 1 1 1 0 0 0 1 0 0 1 1 0 1 0, and the existing 5 bits of the  $Z_n$  code 1 1 1 1 1 0 0 0 1 1 0 1 1 1 0 1 0 1 0 0 0 1 0 1 1 0 0, are also stored in the storage register. After the elapse of transit time  $\tau$ , the 12-bit contents of the  $X_m$ ,  $Y_m$ , and  $Z_m$  decode generators, will match the stored patterns from the encode generators. Figure 5 shows the form factors of these codes in various combinations, as displayed on an oscilloscope. Since the WWV demand pulse started a time interval unit (TIU) at the instant the encoder patterns were stored, and since the comparator unit stopped the TIU at the instant the



7 Bit



15 Bit



31 Bit

For all codes  $\begin{cases} \text{Clockrate} = 4 \text{ Kc} \\ 1 = -6\text{v} \\ 0 = 0\text{v} \end{cases}$

Figure 5a.

$x \oplus y$



Figure 5b.

$x \oplus y$



Figure 5c.



decoder patterns matched the stored patterns, the TIU, a simple fixed frequency counter, determines the transit time in terms of the invariant speed-of-light constant. In the Hybrid application of the TIMER System, the fine stop control of the TIU is controlled by the zero crossing of a relatively high frequency sidetone; the TIMER is used to unambiguously "ready" the TIU for the stopping action of the sidetone.

### 5.1 Correlation Circuit

An important unit in the TIMER System is the correlator which integrates the mod-2 sum of the received code and the decoder code. When the mod-2 sum is a series of approximately equal numbers of 1's and 0's, the codes are uncorrelated; a selectable and relatively long time constant RC circuit averages the -6v and 0 volt levels corresponding respectively to 1's and 0's and indicates the average value of -3 volts. As noted before, the same RC circuit indicates a level of approximately -1.5 volts when one of the short codes is correlated. As each short code is correlated, an automatic shifting process is terminated automatically. After each short code is acquired by this process, a manual switch (which will be automated for the systems used in the tracking network) is thrown to start the automatic acquisition of another short code. Several selectable time constants for integration are available depending upon signal energy levels. In the actual Hybrid System, the lengths of the x, y, and z codes are selectable according to mission requirements for unambiguous ranging; the clock rates, 8, 32, 160, 800, or 4000 cps are also selectable according to range requirements.

The correlation process is, of course, completed before any transit time measurements are made. An automatic lock prevents range data recording unless the correlator unit indicates 100% lock-on.

#### 6. Hybrid System

The Hybrid System is essentially an extension of existing range and range rate units. Two of the major spacecraft ranging systems are the Sidetone type designed and successfully used by the Goddard Space Flight Center and the PN type under development by the Jet Propulsion Laboratories. Since both of these types are described in much detail in a number of the reports given in the Bibliography, the discussions in this report are directed primarily towards describing the technical units employed in the TIMER System. Nevertheless, a few statements about current ranging systems will help to define the Hybrid System in a comparative sense.

The Sidetone ranging system as designed by GSFC employs a number of sidetones whose frequencies are integrally related by a factor of 4 or 5. These sidetones, suitably modulated on a carrier, are transmitted, coherently transponded, and received. After phase-lock loop acquisition of each sidetone in the ground receiver, range measurements are made in essence by measuring the elapsed time for all sidetones transmitted in alternately reversed phases to be received in alternately reversed phases after being transponded in a phase coherent manner in the space-craft. The lowest sidetone employed is selected to be unambiguous for

the distances to be measured (transit time,  $\tau$ , is less than the period,  $T$ , of the lowest frequency sidetone).

The PN ranging system under development by JPL utilizes a PN code imposed upon a clock frequency, equivalent to a single sidetone, and, after phase locked loop acquisition of the clock frequency and correlation of the PN code, range measurements are made, in essence, by determining the phase difference between the transmitted clock and received clock, and by computing the equivalent transit time values of each shift of the short codes which compose the longer acquirable code; after this process, range information is updated by adding in distance changes determined by counting Doppler cycles.

The Hybrid System, in its optimum form, utilizes several sidetones in the manner of the GSFC Range and Range Rate System, and, in addition, imposes a PN code on the lowest sidetone employed to increase non-ambiguous ranging distance. Range measurements are made by direct measurements of the elapsed transit time.

With this orientation, it is noted that the stop pulse action illustrated in the block diagram of Figure 4 is improved by the phase definition of the 20 and 100 Kc sidetones (see Appendix). The Hybrid System thus utilizes sidetone technology and PN technology to determine range by direct transit time measurements. The Hybrid System capitalizes upon both the advantages of sidetone ranging which permits fine distance definition under restricted bandwidth conditions, and upon the advantages

of pseudo random encoding which permits unambiguous ranging at long distances without the need for extremely low frequency sidetones and their associated phase-locked-loop acquisition problems.

The Hybrid System, optimally, utilizes pseudo random encoding of a sidetone, for example 4 Kc, and also utilizes higher sidetones of 20 Kc and 100 Kc for fine distance measurements. It could be used equally well with a single clock frequency, (PN only ranging), but the higher clock frequency necessary for fine ranging, and the higher frequency code would occupy more spectral bandwidth than necessary; longer codes and longer or more complex acquisition processes would also be necessary.

As presently designed, the GSFC Range and Range Rate System solves the ambiguity problem by use of a novel technique of alternately phase reversing each higher frequency transmitted sidetone; this technique permits each half period of a lower frequency sidetone to gate "on" the next higher frequency half period of sidetone at the receiver. By properly arranging a series of flip-flops, the fine determination of range measurement is held to the phase definition of the 100 Kc sidetone which is  $\pm 0.36^\circ$  in the GSFC Range and Range Rate System; this definition is equivalent to a time error of 10 nanoseconds or about five feet of distance. This ultimate distance definition was practically achieved in tracking the Syncom at a range of about 20,000 miles. The Hybrid System retains this capability but utilizes the PN code to fix the time position of the first 4 Kc gate - the 20 Kc and 100 Kc gates then function

as in the present system. In Appendix A, the fundamental units for ranging with the TIMER System are illustrated with their logic equations.

#### 6.1 Cisplanet Ranging

A question arises as to how far the long code is shifted when one of the shorter codes is shifted a given amount. In the TIMER System no computation based on this analysis is employed at cislunar distances. At cisplanet ranging distances some of the TIMER System technology can be profitably employed by utilizing this computation. In the latter case, it is desirable to make range measurements as soon as the ground-satellite-ground loop is filled with RF energy and the decode generator is matched to the received encoded signal (i.e. the received signal is acquired), without waiting the additional time required for a given generator pattern to travel the loop distance. Very briefly, this result can be accomplished by employing the previously described encoder register plus an additional decoder storage register. Range measurements can then be made by measuring the phase difference between encode-decode clocks, and by determining the phase or shift distance of each encode-decode short code one to another. The advantages of this method at cisplanet distances are: one, no additional time beyond acquisition time is required for ranging; two, all ranging measurements are independent; three, code reacquisition is not necessary to obtain independent measurements; and four, sampling rates can be increased as far as practically required.

In order to utilize the cisplanetary techniques outlined above, the contents of the decode generator, as well as the contents of the encode generator, must be stored in a storage register at demand time. Each decoder short code is shifted until the encode-decode short codes match; the number of shifts of each code plus the encode-decode clock phase difference at demand time determine spacecraft range at demand time minus D/C where C is the velocity of light and D is the one-way distance to the spacecraft. Either of the following two equations, derived by means of the Chinese Remainder Theorem of Number Theory, determines the equivalent shift of the long code in terms of the individual shifts of the short codes.

$$-465 \times 2 \text{ (x shift)} - 217 \times 2 \text{ (y shift)}$$

$$+ 105 \times 13 \text{ (z shift)} = (\text{total code shift}) \bmod 3255$$

$$\text{or: } 465 \times 5 \text{ (x shift)} + 217 \times 13 \text{ (y shift)} + 105 \times 13 \text{ (z shift)} \\ = (\text{total code shift}) \bmod 3255$$

It is noted that, the actual computation of distance can be performed at a central computer, instead of at each network station, with little loss in communications efficiency because the number of bits required to transmit the distance information is practically equal to the number of bits required to transmit the code shift and phase information.

For completeness the following fact is noted: if it is desired to shift the long code a given amount, say  $N$  shifts, each short code is shifted  $N_{(\bmod \text{short code})}$ . For example, if the long code is to be shifted an

amount 33, the x code is shifted  $33_{\text{mod } 7}$  or 5, the y code  $33_{\text{mod } 15}$  or 3, and the z code  $33_{\text{mod } 31}$  or 2.

## 6.2 Conclusion

In conclusion, this report has attempted to describe the principles and practical design features of an improved system for spacecraft ranging with a hybrid combination of sidetones and encoded signals. Only by integrating the information presented here, with other information available from the reports listed in the Bibliography, can a complete understanding of all the units necessary for a practical ranging system be obtained. In this brief presentation of principles and practice no deliberate attempt has been made to minimize the essential complexity of spacecraft ranging. By its very nature, spacecraft ranging draws on the ultimate of current technology. This report is intended to enhance this technology by one more contribution, and will have succeeded only when the principles presented here are reduced to practice and are utilized in the range and range rate network.

## APPENDIX I

This Appendix describes the basic, practical, logic circuits for a Hybrid type ranging system employing PN TIMER and Sidetone techniques. Design criteria and operational feasibility are demonstrated.

Figure 1 is a simple block diagram of the TIMER System. Sidetones of 100, 20, and 4 Kc are produced in the Sidetone Generator. The 4 Kc signal is used to drive the Encoder which produces the PN 3255-bit code and is also used as the phase modulated subcarrier for the PN code. The 100 Kc, 20 Kc and PN Code plus 4 Kc are then phase modulated on a carrier and transmitted. The signal is received and coherently transmitted back to the ground by the Transponder. This signal is received by the ground equipment and from it is derived the Decoder Clock frequency (Encoder Clock frequency plus Doppler) and the 100 Kc and 20 Kc Sidetones plus Doppler which are fed to the appropriate phase-locked loops. The Decoder produces a shifted Code identical to that of the Encoder but produces code bits at the clock-plus-Doppler frequency. The Correlator locks the decoder generator to the received code and then by means of the Transit Time circuit, determines the range. Note that the Sidetone Generator, Transmitter, and Receiver equipment shown (but not the PN coders and code modulators and demodulators) already exist as part of the Goddard Range and Range Rate System.

Figure 2 shows the system components in more detail. The TIMER System can be broken down further into the following subsystem designations: the transmitter subsystem which includes the transmitter, the  $W_n$  \* Encoder Generators, the  $W_n$  Code Combiner, and the Mod-2 Modulator; the receiver subsystem which includes the receiver, the  $W_m$  Decoder Generators, the  $W_m$  Code Combiners, and the Countdown Generators; the correlator which includes the Correlation Indicator and Shift Pulse Generator; and the ranging subsystem which includes the Comparator, Stop Pulse Generator, and the Time Interval Unit.

Some of the functional operations of the system components are the following: A local 1 MC oscillator and frequency synthesizer are used to provide frequencies of 100, 20, and 4 Kc. The 4 Kc square wave which is synchronized with the 20 Kc, 100 Kc and WWV frequencies is used to drive the  $W_n$  Encoder Generator, the Mod-2 Modulator, and the Comparator.

The  $W_n$  Encoder Short-Code Generators function to produce the  $X_n$ ,  $Y_n$ , and  $Z_n$  short codes and provide outputs for operating the storage registers in the Comparator, and for combining codes in the  $W_n$  Code Combiner. The Code Combiner provides the output  $X_n \oplus Y_n Z_n$  for operating the Mod-2 Modulator. Additional clock energy, not illustrated, is added to the 4 Kc subcarrier to permit 4 Kc clock phase-lock-loop acquisition in the receiver, independent of code lock-on.

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\*The subscripts n and m are used throughout the Appendix to denote encoder and decoder related items, respectively.

The  $W_m$  Decoder Short-Code Generators function to produce the  $X_m$ ,  $Y_m$ , and  $Z_m$  short codes and outputs for operating the Comparator gates, the  $W_m$  Code Combiners, and the Countdown Generators. The  $W_m$  Code Combiner outputs,  $X \oplus YZ$ ,  $X_m \oplus Y_m$ , and  $X_m \oplus Z_m$  are used for correlation indication. The Countdown Generators produce countdown pulses of 3255:1, 217:1, and 105:1 to provide different shift rates for the Shift Pulse Generator.

The Correlation Indicator serves to detect and display correlation of the received code with  $W_m$ .

Correlation is obtained by shifting  $W_m$  with respect to the received code by means of extra shift pulses (added to the clock plus Doppler shift pulses) from the Shift Pulse Generator.

The Comparator is used to compare the transmitted code with the received code thereby providing the time basis for range determination; the Comparator also serves to activate the Stop Pulse Generator. Actual range is determined by the Time Interval Unit which is activated by a WWV demand pulse and deactivated by the Stop Pulse Generator.

The sequence of operations is as follows: The output of the Mod-2 Modulator,  $W_n \oplus C_1$ , where  $C_1$  is the 4 Kc System Clock, together with the 100 and 20 Kc frequencies, is phase-modulated on a carrier and transmitted.

The complex signal is coherently transponded and received by existing equipment in the Goddard RARR system and, after proper conditioning,

is detected by the 100, 20, and 4 Kc phase locked loops. Each loop contains the particular sidetone plus its doppler frequency. The received 4 Kc Clock plus Doppler constitutes the Decoder clock; this signal also contains the received PN code information. Initially, the received code and the local code generated by the Decoder generators,  $W_m$ , are uncorrelated, i.e., are out of phase by an undetermined number of bits.

The correlation condition is detected and displayed by the correlation indicator, which determines sequentially the correlation levels of the decoder  $X_m$ ,  $Y_m$ , and  $Z_m$  short codes, with respect to the total received combined code. The short codes are actually correlated as  $X_m$ ,  $X_m \oplus Y_m$ ,  $X_m \oplus Z_m$ , and  $X_m \oplus Y_m Z_m$ , in sequence.

The shift pulse generator shown is used to shift, separately, the  $X_m$ ,  $Y_m$ , and  $Z_m$  short codes. When one of these short codes is correlated with its component in the received code, the Shift Pulse Generator is automatically turned off by a pulse generated by the Correlation Indicator. This allows the shift pulse to be directed by manual switching to the other  $W_m$  short code generators. Because of this self-turn-off feature, no shift pulses are generated after complete correlation is obtained.

When complete correlation exists and on demand from WWV, the Time Interval Unit is activated; at the same time the 12-bit Encoder word is stored in the registers of the Comparator. When the outputs of the registers of the Decoder generators (running synchronous with the

received code) match the stored code, a stop pulse is generated which readies the Time Interval Unit for the stop command from the highest sidetone used. The time interval reading obtained is the range in transit time units.

Figure 3 shows the Encoder-Decoder short code generators. The design of each is such that a maximal linear short code is generated, i.e., a code of  $2^n - 1$  bits is obtained, where  $n$  is the number of stages in the shift register. Thus the X, Y, and Z short codes contain, respectively, 7, 15, and 31 bits. These generators are implemented with modulo-2 (exclusive "or") logic by means of the gated feedback from appropriate stages of the register. At (4), a logical "1" will be generated when the outputs of each stage differ and a logical "0" when the outputs are alike (either two "1's" or two "0's"). Without input (3) (a self-starting mechanism) the outputs at (4) are represented by the functions:

$F(x) = b_x \oplus c_x$ ,  $F(y) = c_y \oplus d_y$ ,  $F(z) = c_z \oplus e_z$ , where  $F(x)$ ,  $F(y)$ ,  $F(z)$  represent the logic functions, respectively of the x, y, and z short code generators, and  $b_x$ ,  $c_x$ ,  $c_y$ ,  $d_y$ ,  $c_z$ , and  $e_z$  represent outputs of particular stages of those generators. Note that for the maximal linear Z-code, outputs c and e (stages 3 and 5) are tapped rather than d and e, (the last two stages).

For system reliability, a self-starter is incorporated into the design of each Short Code Generator to assure code generation each time the system is turned on. A logical "1" will be generated by the self-starter at (3) for all conditions except when the reset outputs ( $\bar{a}$ ,  $\bar{b}$ ,  $\bar{c}$ ) of

the generators are all in the "1" state (or the set outputs are all "0's").

Then a logical "0" is generated at (3) which provides proper gating at gate (4). Without this feature the codes would not be generated if all stages were in the zero state at turn-on. With the self-starter, the functions of X, Y, and Z at (4) are:

$$F(x) = b_x \oplus c_x + \bar{b}_x \cdot \bar{c}_x, \quad F(y) = c_y \oplus d_y + \bar{a}_y \cdot \bar{b}_y \cdot \bar{c}_y \cdot \bar{d}_y, \quad F(z) = c_z \oplus e_z + \bar{a}_z \cdot \bar{b}_z \cdot \bar{c}_z \cdot \bar{d}_z \cdot \bar{e}_z.$$

Figure 4.1 and 4.2 show the  $W_m$  (Decoder) Sub-Code Combiners.

Each Sub-Code combiner adds, modulo-2, the  $X_m$  short code with one of the other short codes. The output at 1.3 is the  $X_m \oplus Z_m$  sub-code containing 217 bits, i.e., the  $X_m$  short code length (7 bits) times the  $Z_m$  code length (31 bits). The output at 2.3 is the  $X_m \oplus Y_m$  sub-code containing 105 bits, i.e., the  $X_m$  short code length times the  $Y_m$  short code length ( $7 \times 15$ ).

The long-code combiner shown in Figure 4.3 illustrates the circuitry used to combine the X, Y, and Z codes into the long code  $X \oplus Y \oplus Z$ . This diagram is applicable to both the encoder combiner which generates  $W_n$ , and the decoder combiner which generates  $W_m$ .

The long-code combiner generates by simple logical addition and modulo-2 logic the combination of the three short code generators. The output at 3.5 is the long code  $X_n \oplus Y_n Z_n$  (for the encoder) and  $X_m \oplus Y_m Z_m$  (for the decoder) containing 3255 bits. i.e., the product of the X, Y, and Z short code lengths,  $7 \times 15 \times 31$ .

The Mod-2 Modulator in Figure 5 combines, modulo-2, the clock, C1, with the long code,  $W_n = X_n \oplus Y_n Z_n$ , giving at (3)  $W_n \oplus C1$ . Additional

Clock energy is added (not shown) to permit received clock phase-lock-on independent of code correlation.

In Figure 6, the Countdown Generators generate a countdown pulse of 3255:1 at (6) each time the code is repeated and all generators contain a logical "1" in the set position; a countdown pulse of 105:1 at (3) when all the set outputs of the  $X_m$  and  $Y_m$  generators are in the logical "1" position; and a countdown pulse of 217:1 at (8) when all the set outputs of the  $X_m$  and  $Z_m$  generators are in the logical "1" position.

Figure 7 shows both the Correlation Indicator and the Shift Pulse Generator. By combining, separately,  $X_m$ ,  $X_m \oplus Y_m$ ,  $X_m \oplus Z_m$  with  $W_R$  (the received code), mod-2, and then integrating, correlation of each  $W_m$ -short code with the  $W_R$ -long code can be detected and displayed on the meter at (4). When the codes are not correlated, the voltage reading at (4) is approximately -3 volts. When one of the  $W_m$ -short codes is correlated with its corresponding component in the received  $W_R$ -long-code, the voltage rises to approximately -1.5 volts. Note that on complete correlation of  $W_m$  with received  $W_R$ , the voltage reading at (4) is 0 V, (because with mod-2 logic, all ones or all zeros gives an output of 0 volts.)

The Schmitt Trigger, sensitive to the change in Voltage (from -3v to -1.5 volts), triggers gate (5) which then turns off gate (10), stopping the shift pulse (9). The output at (12) then changes from  $F(12) = CD \cdot \bar{I} + C1$  to  $F(12) = C1$  (where  $CD$  = Countdown,  $I$  = integration, and  $C1$  = clock).

At complete correlation, the Decoder runs synchronously with the received code at the received clock-plus-Doppler rate.

The Comparator, Stop Pulse Generator, and Time Interval Unit shown in Figure 8 function to provide a range reading.

On demand from WWV, the TIU is activated and simultaneously gate (12) is triggered, stopping the system clock input. The transmitted code (the 12-bit Encoder word) is stored in the registers of the Comparator. The demand pulse is timed to occur on the negative going portion of one of the 4 Kc square wave clock cycles or 125 microseconds (1/2 period) after the previous positive going portion has shifted both the short-code generators and Storage Registers. This technique insures that the Storage Registers contain the proper transmitted code, i.e., the three, four, and five-bit Encoder words. The next shift changes the contents of the generators but does not change the contents of the registers. This shift occurs 125 microseconds after demand time, on the next positive going portion of the 4 Kc square wave. Note that during the 125 microsecond period previous to demand time, the Encoder three, four, and five-bit words have been "on the air." The total transit time  $\tau$ , is, therefore, the measured transit time,  $\tau'$ , plus 125 microseconds.

By means of the Comparator gates, the locally generated model of the received code is compared with the stored code. When matched, a reset pulse is generated which turns off  $FF_1$ . Simultaneously,  $FF_2$  is turned on. When the positive going portion of the 20 Kc frequency tone

occurs,  $FF_2$  is turned off. At the same time,  $FF_3$  is turned on. In the manner described above, the 100 Kc frequency tone will turn off  $FF_3$ , and simultaneously the TIU will be deactivated. A constant time interval consisting of the sum of the half periods of the 100, and 20 Kc side-tones is included in the above transit time reading. This constant time is subtracted to obtain the true distance in transit time units.

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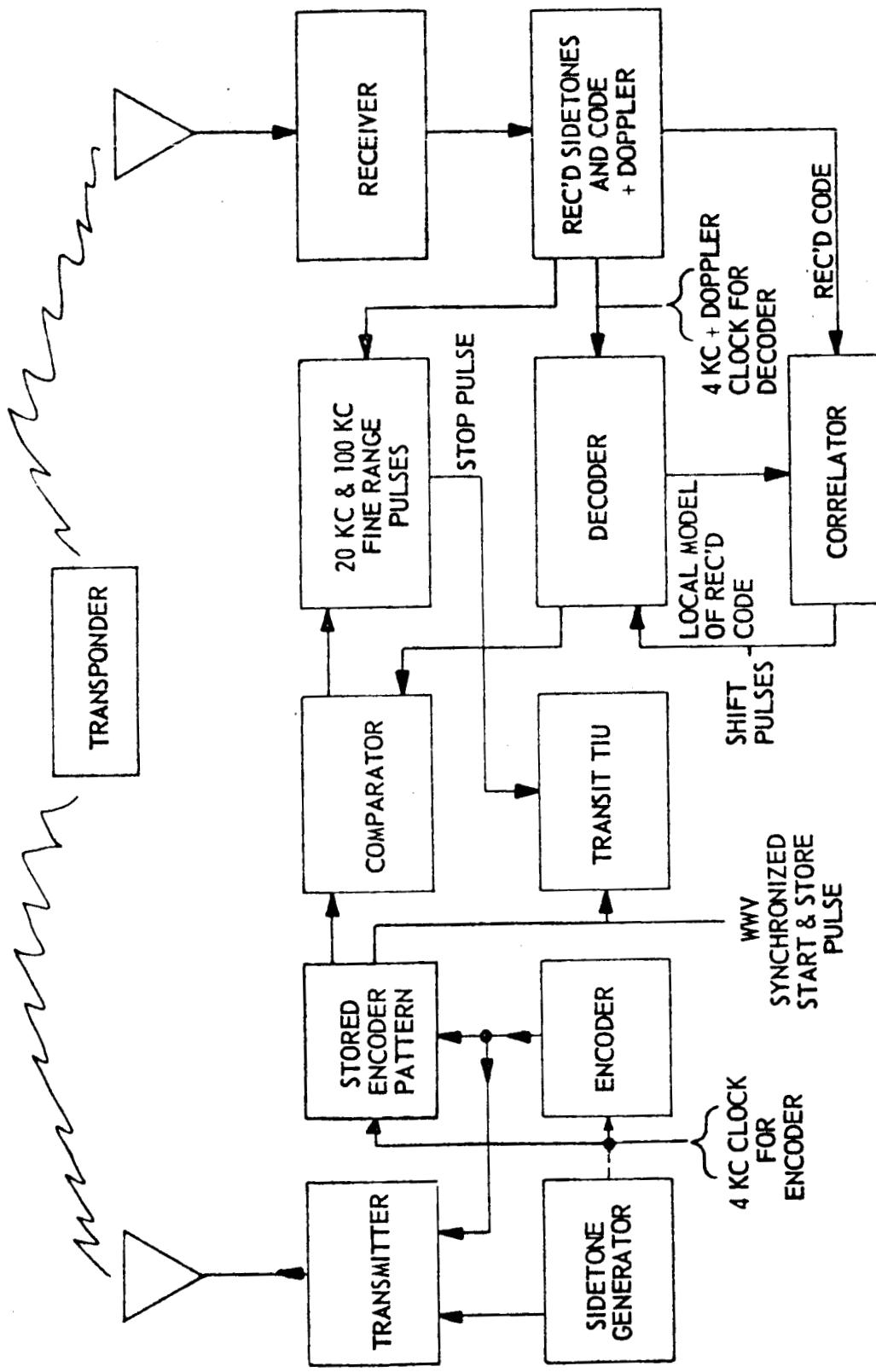


Figure 1. Simplified System Block Diagram

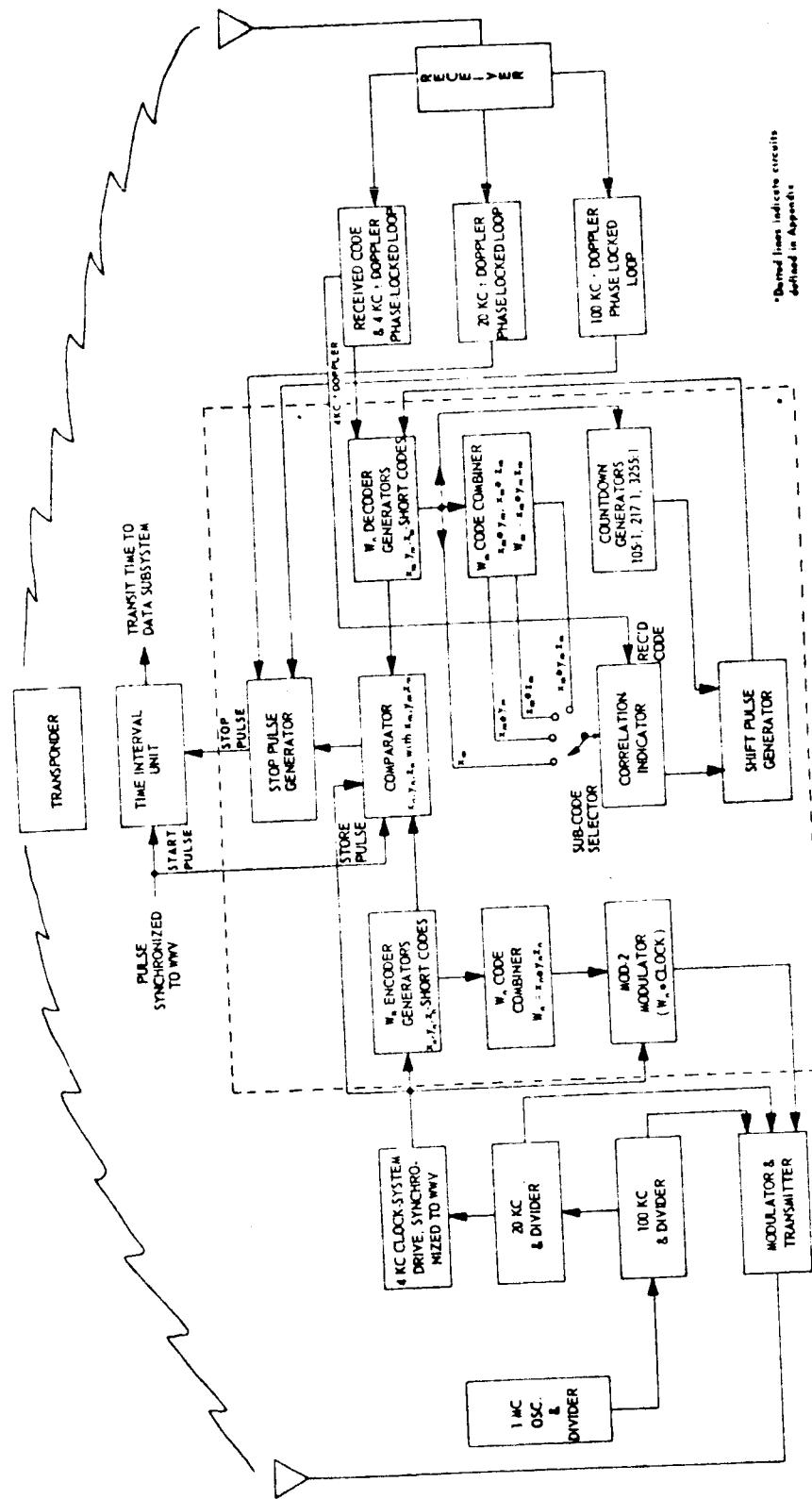
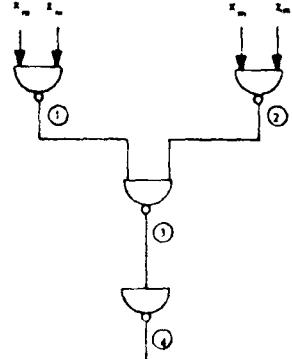
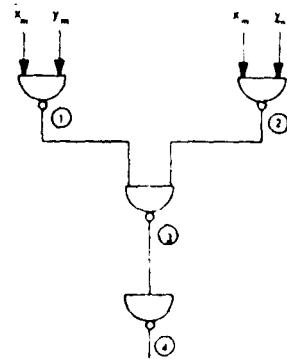


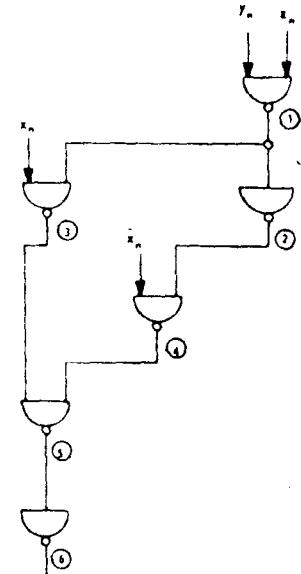
Figure 2. System Block Diagram



### 1. $x_m \oplus z_m$ SUB-CODE COMBINER



## 2. $x_n \oplus y_n$ SUB-CODE COMBINER



3.  $x + y - z$  LONG CODE COMBINER  
SHOWN FOR ENCODER. (DUPLI-  
cate decoder diagram not  
shown).

**SUB-CODE COMBINER**

- 1.1.  $F_{m(1)} = x_m \cdot z_m$
- 1.2.  $F_{m(2)} = \overline{x_m \cdot z_m}$
- 1.3.  $F_{m(3)} = (x_m + z_m) \cdot (\overline{x_m} + \overline{z_m})$
- 1.4.  $F_{m(4)} = \overline{x_m \cdot z_m}$

**Legend:** See Fig. 3  
Letters n and m refer to encoder, decoder related functions, respectively.

**x<sub>n</sub> • y<sub>n</sub> SUB-CODE COMBINER**

- 2.1.  $F_{n(1)} = \overline{x_n \cdot y_n}$
- 2.2.  $F_{n(2)} = \overline{x_n + y_n}$
- 2.3.  $F_{n(3)} = (\overline{x_n} \cdot y_n) + (x_n \cdot \overline{y_n})$

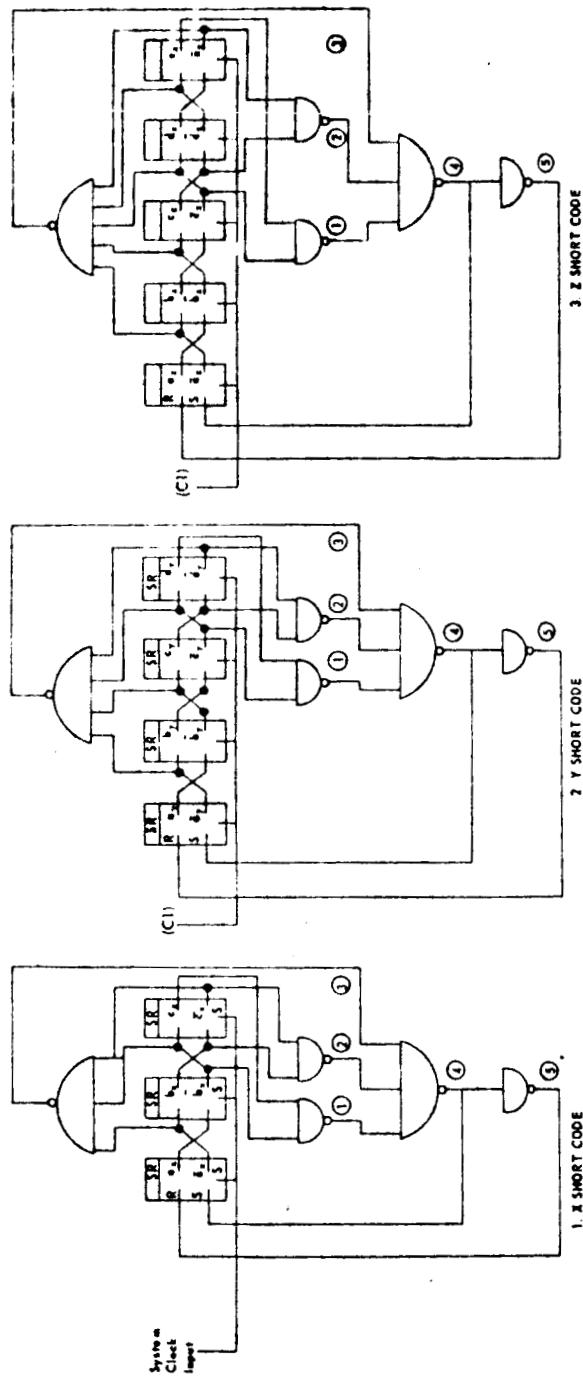
$= x_n \oplus y_n$

- 2.4.  $F_{n(4)} = \overline{x_n \oplus y_n}$

**LONG CODE COMBINER**

- 3.1.  $F_{n+1} = \overline{y_n \cdot z_n}$
- 3.2.  $F_{n+2} = y_n \cdot z_n$
- 3.3.  $F_{n+3} = \overline{x_n \cdot (y_n \cdot z_n)}$
- 3.4.  $F_{n+4} = \overline{x_n \cdot (y_n \cdot z_n)}$
- 3.5.  $F_{n+5} = [x_n \cdot (y_n \cdot z_n)] \cdot \overline{[x_n \cdot (y_n \cdot z_n)]}$   
 $= x_n \circ y_n \cdot z_n$
- 3.6.  $F_{n+6} = \overline{x_n \circ y_n \cdot z_n}$

Figure 4.  $W_m$  Sub-Code Combiners and  $W_n - W_m$  Code Combiner.



#### 1. X-SHORT CODE

$$\begin{aligned} 1.1. \quad F_{(1)} &= \overline{\overline{c}_1 \cdot c_2} \\ 1.2. \quad F_{(2)} &= b_1 \cdot \overline{\overline{c}_1 \cdot c_2} \\ 1.3. \quad F_{(3)} &= \overline{\overline{a}_1 \cdot b_1} \cdot \overline{\overline{c}_1 \cdot d_1} \\ 1.4. \quad F_{(4)} &= F_{(1)} \end{aligned}$$

$$= (b_2 \cdot c_2) \cdot (b_3 \cdot c_3) \cdot \overline{a_1} \cdot \overline{b_1} \cdot \overline{c_1} \cdot d_1$$

$$= b_2 \cdot c_2 + \overline{b_2} \cdot \overline{b_3} \cdot \overline{c_2} \cdot \overline{c_3}$$

$$1.5. \quad F_{(5)} = b_1 \cdot \overline{c_1 \cdot d_1} \cdot \overline{\overline{b}_1 \cdot \overline{c}_1 \cdot \overline{d}_1}$$

#### 2. Y-SHORT CODE

$$\begin{aligned} 2.1. \quad F_{(1)} &= \overline{\overline{c}_2 \cdot d_1} \\ 2.2. \quad F_{(2)} &= c_2 \cdot \overline{\overline{c}_2 \cdot d_1} \\ 2.3. \quad F_{(3)} &= \overline{\overline{b}_2 \cdot c_2} \cdot \overline{\overline{c}_2 \cdot d_1} \\ 2.4. \quad F_{(4)} &= F_{(2)} \end{aligned}$$

$$= (c_2 \cdot d_1) \cdot (c_2 \cdot d_1) \cdot \overline{a_1} \cdot \overline{b_1} \cdot \overline{c_1} \cdot d_1$$

$$= c_2 \cdot d_1 + \overline{b_2} \cdot \overline{b_3} \cdot \overline{c_2} \cdot \overline{d_1}$$

$$2.5. \quad F_{(5)} = c_2 \cdot d_1 \cdot \overline{a_1} \cdot \overline{b_1} \cdot \overline{c_1} \cdot \overline{d_1}$$

#### 3. Z-SHORT CODE

$$\begin{aligned} 3.1. \quad F_{(1)} &= \overline{\overline{c}_1 \cdot \overline{c}_2} \\ 3.2. \quad F_{(2)} &= \overline{\overline{c}_1 \cdot \overline{c}_2} \cdot \overline{\overline{c}_1 \cdot \overline{c}_2} \\ 3.3. \quad F_{(3)} &= \overline{\overline{b}_1 \cdot \overline{b}_2} \cdot \overline{\overline{c}_1 \cdot \overline{c}_2} \cdot \overline{\overline{d}_1 \cdot \overline{d}_2} \\ 3.4. \quad F_{(4)} &= F_{(1)} \end{aligned}$$

$$= (c_1 \cdot \overline{c}_2) \cdot (\overline{c}_1 \cdot \overline{c}_2) \cdot \overline{a_1} \cdot \overline{b_1} \cdot \overline{c_1} \cdot \overline{d}_1$$

$$= c_1 \cdot \overline{c}_2 + \overline{b}_1 \cdot \overline{b}_2 \cdot \overline{c}_1 \cdot \overline{d}_1$$

$$3.5. \quad F_{(5)} = c_1 \cdot \overline{c}_1 \cdot \overline{a_1} \cdot \overline{b_1} \cdot \overline{c_1} \cdot \overline{d}_1$$

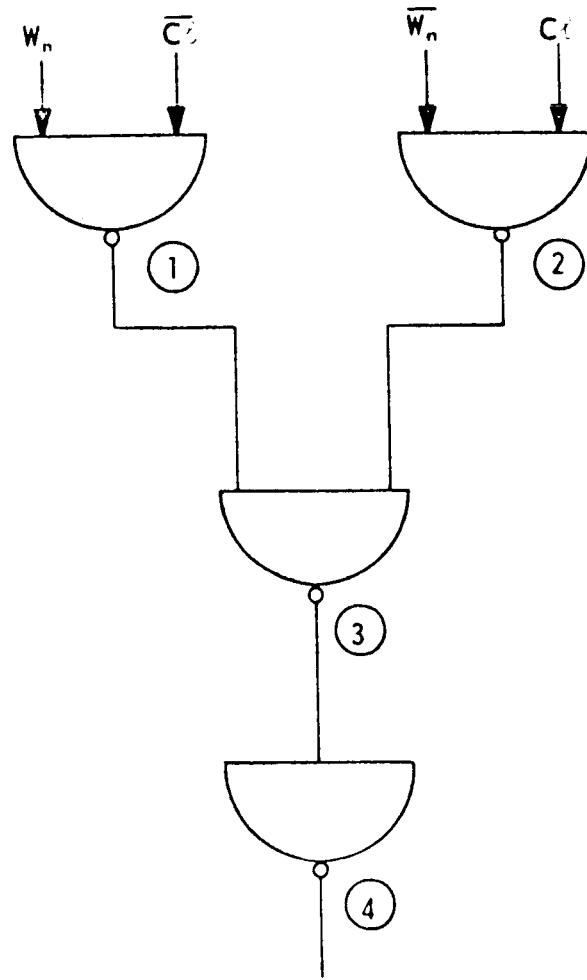
**Legend:**  $F_{(1)}, F_{(2)}, \dots$  refer to the existing functions at the related points designated by a circled number on the above logic diagram.

$F_{(x)}, F_{(y)}, \dots$  refer to the functions which generate the encoding decoding PN codes  $x, y, \dots$  respectively.

Letters  $a, b, \dots$  refer to particular shift register stages.

The subscripts in terms  $c_1, c_2, \dots$  refer to shift registers which are associated with codes  $x, y, \dots$  respectively.

Figure 3. Encoder - Decoder Generators



$$1. F_{n(1)} = \overline{W_n \cdot \bar{C1}}$$

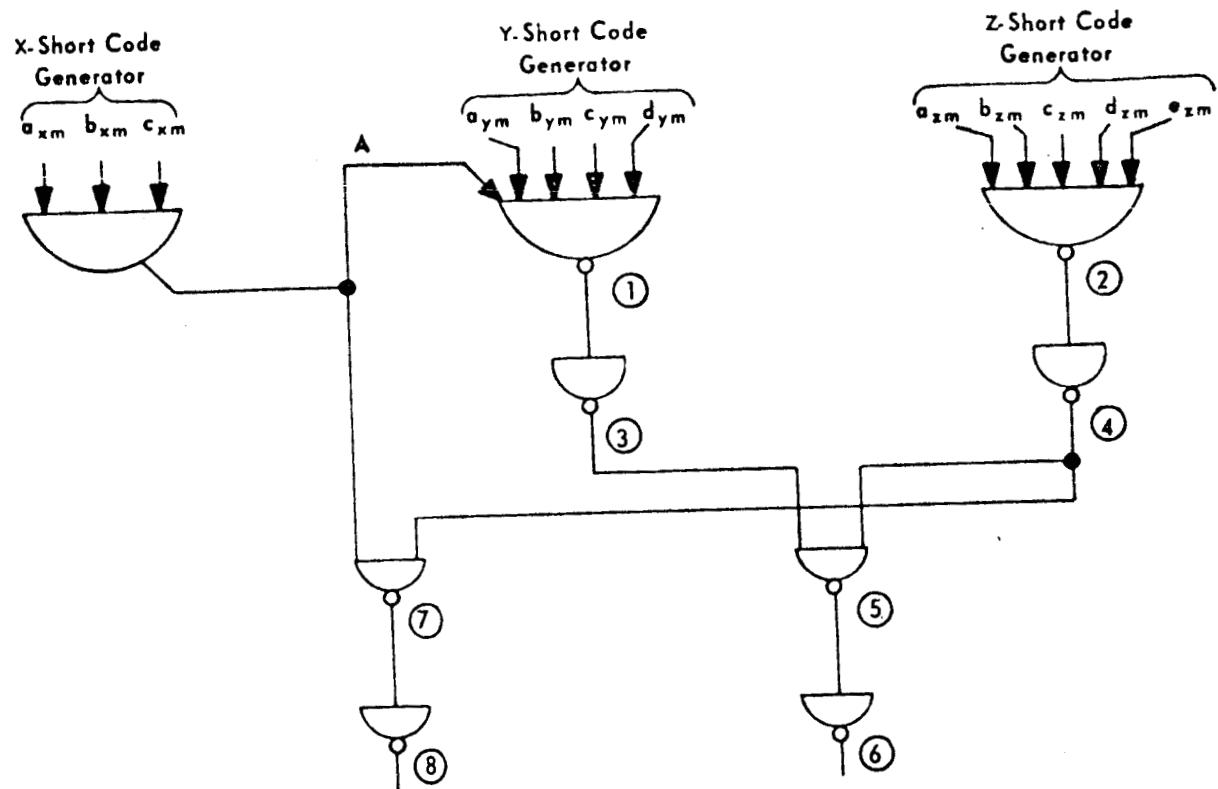
$$2. F_{n(2)} = \overline{\overline{W_n} \cdot C1}$$

$$3. F_{n(3)} = (\overline{W_n \cdot \bar{C1}}) \cdot (\overline{\overline{W_n} \cdot C1}) \\ = W_n \oplus C1$$

$$4. F_{n(4)} = \overline{W_n \oplus C1}$$

Legend: See Figures 3 and 4  
 $C1$  = System clock input  
 $W_n$  = decoder long code

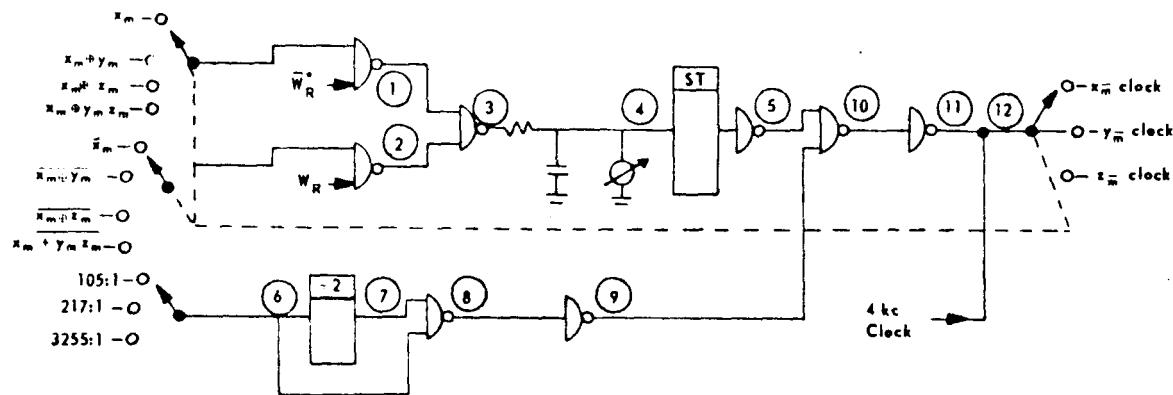
Figure 5. MOD-2 Modulator



Let  $A = a_{xm} \cdot b_{xm} \cdot c_{xm}$   
 $B = a_{ym} \cdot b_{ym} \cdot c_{ym} \cdot d_{ym}$   
 $C = a_{zm} \cdot b_{zm} \cdot c_{zm} \cdot d_{zm} \cdot e_{zm}$

1.  $F_{m(1)} = \overline{A \cdot B}$
2.  $F_{m(2)} = \overline{C}$
3.  $F_{m(3)} = A \cdot B = \text{Countdown of } 105:1$
4.  $F_{m(4)} = C$
5.  $F_{m(5)} = \overline{A \cdot B \cdot C}$
6.  $F_{m(6)} = A \cdot B \cdot C = \text{Countdown of } 3255:1$
7.  $F_{m(7)} = \overline{A \cdot C}$
8.  $F_{m(8)} = A \cdot C = \text{Countdown of } 217:1$

Figure 6. Countdown Generators

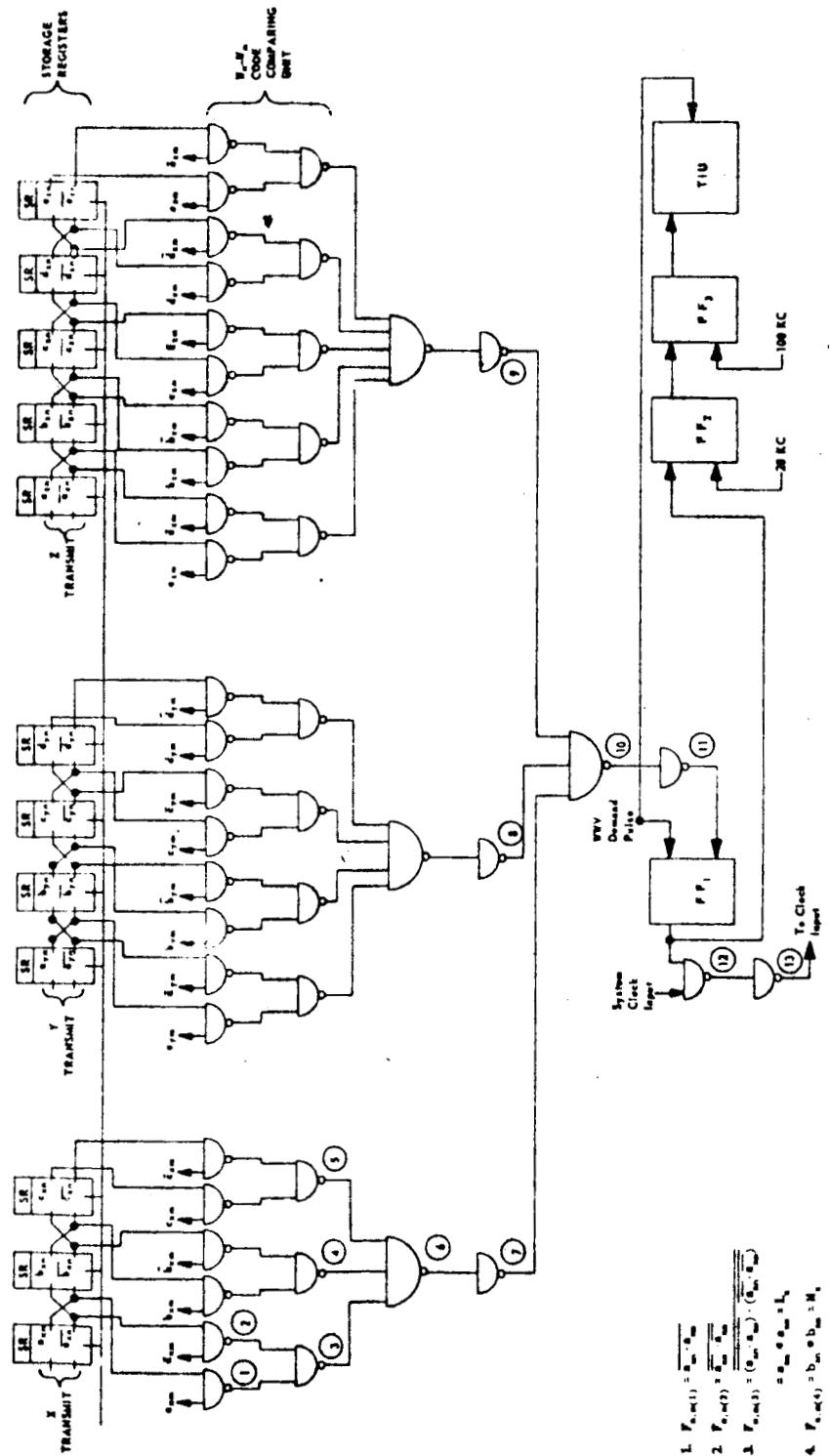


\*Subscript R designates received code

1.  $F_{R,m}(1) = \overline{W_R \cdot W_m}$
2.  $F_{R,m}(2) = \overline{W_R \cdot \overline{W_m}}$
3.  $F_{R,m}(3) = (\overline{W_R \cdot W_m}) \cdot (\overline{W_R \cdot \overline{W_m}}) = W_R \oplus W_m$
4.  $F_{R,m}(4) = I$
5.  $F_{R,m}(5) = \overline{I}$
6.  $F_m(6) = CD$
7.  $F_m(7) = CD_2$
8.  $F_m(8) = \overline{CD_2} \cdot CD$
9.  $F_m(9) = CD_2 \cdot CD = CD_2$
10.  $F_{R,m}(10) = \overline{CD_2 \cdot I}$
11.  $F_{R,m}(11) = CD_2 \cdot \overline{I}$
12.  $F_{R,m}(12) = CD_2 \cdot \overline{I} \cdot C1$

Legend: Subscript R refers to received code  
 $I$  = Continuous correlation  
 $CD$  = Countdown pulse  
 $CD_2$  = Countdown pulse, divided by  
two (used as extra shift pulses  
added to clock shift pulses)

Figure 7. Correlation Indicator and Shift Pulse Generator



**Figure 8.** Comparator and Stop Pulse Generator

TABLE 3  
MOLAL THERMODYNAMIC FUNCTIONS FOR L-VALINE  
 $(\text{CH}_3)_2\text{CH}(\text{NH}_2)\text{CHCOOH}$   
SOLID PHASE

GRAM MOLECULAR WT. = 117.14892 GRAMS  
T DEG K = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

T DEG K	$C_p^C$ CAL/DEG	$(H_{T=0}^0 - H_0^0)$ CAL	$(H_{T=0}^0 - H_0^0)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(\dot{Q}_{T=0}^0 - H_0^0)$ CAL	$-(G_{T=0}^0 - H_0^0)/T$ CAL/DEG
273.15	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
283.15	0.9921	0.0000	0.0000	0.0000	0.0000	0.0000
293.15	0.9848	0.0000	0.0000	0.0000	0.0000	0.0000
303.15	0.9772	0.0000	0.0000	0.0000	0.0000	0.0000
313.15	0.9695	0.0000	0.0000	0.0000	0.0000	0.0000
323.15	0.9616	0.0000	0.0000	0.0000	0.0000	0.0000
333.15	0.9534	0.0000	0.0000	0.0000	0.0000	0.0000
343.15	0.9452	0.0000	0.0000	0.0000	0.0000	0.0000
353.15	0.9369	0.0000	0.0000	0.0000	0.0000	0.0000
363.15	0.9285	0.0000	0.0000	0.0000	0.0000	0.0000
373.15	0.9200	0.0000	0.0000	0.0000	0.0000	0.0000
383.15	0.9114	0.0000	0.0000	0.0000	0.0000	0.0000
393.15	0.9027	0.0000	0.0000	0.0000	0.0000	0.0000
403.15	0.8939	0.0000	0.0000	0.0000	0.0000	0.0000
413.15	0.8849	0.0000	0.0000	0.0000	0.0000	0.0000
423.15	0.8758	0.0000	0.0000	0.0000	0.0000	0.0000
433.15	0.8666	0.0000	0.0000	0.0000	0.0000	0.0000
443.15	0.8573	0.0000	0.0000	0.0000	0.0000	0.0000
453.15	0.8479	0.0000	0.0000	0.0000	0.0000	0.0000
463.15	0.8384	0.0000	0.0000	0.0000	0.0000	0.0000
473.15	0.8289	0.0000	0.0000	0.0000	0.0000	0.0000
483.15	0.8193	0.0000	0.0000	0.0000	0.0000	0.0000
493.15	0.8096	0.0000	0.0000	0.0000	0.0000	0.0000
503.15	0.7998	0.0000	0.0000	0.0000	0.0000	0.0000
513.15	0.7899	0.0000	0.0000	0.0000	0.0000	0.0000
523.15	0.7799	0.0000	0.0000	0.0000	0.0000	0.0000
533.15	0.7698	0.0000	0.0000	0.0000	0.0000	0.0000
543.15	0.7596	0.0000	0.0000	0.0000	0.0000	0.0000
553.15	0.7494	0.0000	0.0000	0.0000	0.0000	0.0000
563.15	0.7391	0.0000	0.0000	0.0000	0.0000	0.0000
573.15	0.7288	0.0000	0.0000	0.0000	0.0000	0.0000
583.15	0.7184	0.0000	0.0000	0.0000	0.0000	0.0000
593.15	0.7079	0.0000	0.0000	0.0000	0.0000	0.0000
603.15	0.6974	0.0000	0.0000	0.0000	0.0000	0.0000
613.15	0.6868	0.0000	0.0000	0.0000	0.0000	0.0000
623.15	0.6761	0.0000	0.0000	0.0000	0.0000	0.0000
633.15	0.6653	0.0000	0.0000	0.0000	0.0000	0.0000
643.15	0.6544	0.0000	0.0000	0.0000	0.0000	0.0000
653.15	0.6434	0.0000	0.0000	0.0000	0.0000	0.0000
663.15	0.6323	0.0000	0.0000	0.0000	0.0000	0.0000
673.15	0.6212	0.0000	0.0000	0.0000	0.0000	0.0000
683.15	0.6101	0.0000	0.0000	0.0000	0.0000	0.0000
693.15	0.5989	0.0000	0.0000	0.0000	0.0000	0.0000
703.15	0.5877	0.0000	0.0000	0.0000	0.0000	0.0000
713.15	0.5765	0.0000	0.0000	0.0000	0.0000	0.0000
723.15	0.5653	0.0000	0.0000	0.0000	0.0000	0.0000
733.15	0.5541	0.0000	0.0000	0.0000	0.0000	0.0000
743.15	0.5429	0.0000	0.0000	0.0000	0.0000	0.0000
753.15	0.5317	0.0000	0.0000	0.0000	0.0000	0.0000
763.15	0.5204	0.0000	0.0000	0.0000	0.0000	0.0000
773.15	0.5091	0.0000	0.0000	0.0000	0.0000	0.0000
783.15	0.4978	0.0000	0.0000	0.0000	0.0000	0.0000
793.15	0.4864	0.0000	0.0000	0.0000	0.0000	0.0000
803.15	0.4751	0.0000	0.0000	0.0000	0.0000	0.0000
813.15	0.4637	0.0000	0.0000	0.0000	0.0000	0.0000
823.15	0.4524	0.0000	0.0000	0.0000	0.0000	0.0000
833.15	0.4410	0.0000	0.0000	0.0000	0.0000	0.0000
843.15	0.4297	0.0000	0.0000	0.0000	0.0000	0.0000
853.15	0.4183	0.0000	0.0000	0.0000	0.0000	0.0000
863.15	0.4069	0.0000	0.0000	0.0000	0.0000	0.0000
873.15	0.3955	0.0000	0.0000	0.0000	0.0000	0.0000
883.15	0.3841	0.0000	0.0000	0.0000	0.0000	0.0000
893.15	0.3727	0.0000	0.0000	0.0000	0.0000	0.0000
903.15	0.3613	0.0000	0.0000	0.0000	0.0000	0.0000
913.15	0.3500	0.0000	0.0000	0.0000	0.0000	0.0000
923.15	0.3386	0.0000	0.0000	0.0000	0.0000	0.0000
933.15	0.3272	0.0000	0.0000	0.0000	0.0000	0.0000
943.15	0.3158	0.0000	0.0000	0.0000	0.0000	0.0000
953.15	0.3044	0.0000	0.0000	0.0000	0.0000	0.0000
963.15	0.2930	0.0000	0.0000	0.0000	0.0000	0.0000
973.15	0.2816	0.0000	0.0000	0.0000	0.0000	0.0000
983.15	0.2702	0.0000	0.0000	0.0000	0.0000	0.0000
993.15	0.2588	0.0000	0.0000	0.0000	0.0000	0.0000
1003.15	0.2474	0.0000	0.0000	0.0000	0.0000	0.0000
1013.15	0.2360	0.0000	0.0000	0.0000	0.0000	0.0000
1023.15	0.2246	0.0000	0.0000	0.0000	0.0000	0.0000
1033.15	0.2132	0.0000	0.0000	0.0000	0.0000	0.0000
1043.15	0.2018	0.0000	0.0000	0.0000	0.0000	0.0000
1053.15	0.1904	0.0000	0.0000	0.0000	0.0000	0.0000
1063.15	0.1790	0.0000	0.0000	0.0000	0.0000	0.0000
1073.15	0.1676	0.0000	0.0000	0.0000	0.0000	0.0000
1083.15	0.1562	0.0000	0.0000	0.0000	0.0000	0.0000
1093.15	0.1448	0.0000	0.0000	0.0000	0.0000	0.0000
1103.15	0.1334	0.0000	0.0000	0.0000	0.0000	0.0000
1113.15	0.1220	0.0000	0.0000	0.0000	0.0000	0.0000
1123.15	0.1106	0.0000	0.0000	0.0000	0.0000	0.0000
1133.15	0.0992	0.0000	0.0000	0.0000	0.0000	0.0000
1143.15	0.0878	0.0000	0.0000	0.0000	0.0000	0.0000
1153.15	0.0764	0.0000	0.0000	0.0000	0.0000	0.0000
1163.15	0.0650	0.0000	0.0000	0.0000	0.0000	0.0000
1173.15	0.0536	0.0000	0.0000	0.0000	0.0000	0.0000
1183.15	0.0422	0.0000	0.0000	0.0000	0.0000	0.0000
1193.15	0.0308	0.0000	0.0000	0.0000	0.0000	0.0000
1203.15	0.0194	0.0000	0.0000	0.0000	0.0000	0.0000
1213.15	0.0080	0.0000	0.0000	0.0000	0.0000	0.0000
1223.15	-0.0234	0.0000	0.0000	0.0000	0.0000	0.0000
1233.15	-0.1368	0.0000	0.0000	0.0000	0.0000	0.0000
1243.15	-0.2502	0.0000	0.0000	0.0000	0.0000	0.0000
1253.15	-0.3636	0.0000	0.0000	0.0000	0.0000	0.0000
1263.15	-0.4770	0.0000	0.0000	0.0000	0.0000	0.0000
1273.15	-0.5904	0.0000	0.0000	0.0000	0.0000	0.0000
1283.15	-0.7038	0.0000	0.0000	0.0000	0.0000	0.0000
1293.15	-0.8172	0.0000	0.0000	0.0000	0.0000	0.0000
1303.15	-0.9306	0.0000	0.0000	0.0000	0.0000	0.0000
1313.15	-1.0439	0.0000	0.0000	0.0000	0.0000	0.0000
1323.15	-1.1573	0.0000	0.0000	0.0000	0.0000	0.0000
1333.15	-1.2707	0.0000	0.0000	0.0000	0.0000	0.0000
1343.15	-1.3841	0.0000	0.0000	0.0000	0.0000	0.0000
1353.15	-1.4975	0.0000	0.0000	0.0000	0.0000	0.0000
1363.15	-1.6109	0.0000	0.0000	0.0000	0.0000	0.0000
1373.15	-1.7243	0.0000	0.0000	0.0000	0.0000	0.0000
1383.15	-1.8377	0.0000	0.0000	0.0000	0.0000	0.0000
1393.15	-1.9511	0.0000	0.0000	0.0000	0.0000	0.0000
1403.15	-2.0645	0.0000	0.0000	0.0000	0.0000	0.0000
1413.15	-2.1779	0.0000	0.0000	0.0000	0.0000	0.0000
1423.15	-2.2913	0.0000	0.0000	0.0000	0.0000	0.0000
1433.15	-3.4047	0.0000	0.0000	0.0000	0.0000	0.0000
1443.15	-4.5181	0.0000	0.0000	0.0000	0.0000	0.0000
1453.15	-5.6315	0.0000	0.0000	0.0000	0.0000	0.0000
1463.15	-6.7449	0.0000	0.0000	0.0000	0.0000	0.0000
1473.15	-7.8583	0.0000	0.0000	0.0000	0.0000	0.0000
1483.15	-8.9717	0.0000	0.0000	0.0000	0.0000	0.0000
1493.15	-10.0851	0.0000	0.0000	0.0000	0.0000	0.0000
1503.15	-11.1985	0.0000	0.0000	0.0000	0.0000	0.0000
1513.15	-12.3119	0.0000	0.0000	0.0000	0.0000	0.0000
1523.15	-13.4253	0.0000	0.0000	0.0000	0.0000	0.0000
1533.15	-14.5387	0.0000	0.0000	0.0000	0.0000	0.0000
1543.15	-15.6521	0.0000	0.0000	0.0000	0.0000	0.0000
1553.15	-16.7655	0.0000	0.0000	0.0000	0.0000	0.0000
1563.15	-17.8789	0.0000	0.0000	0.0000	0.0000	0.0000
1573.15	-18.9923	0.0000	0.0000	0.0000	0.0000	0.0000
1583.15	-20.1057	0.0000	0.0000	0.0000	0.0000	0.0000
1593.15	-21.2191	0.0000	0.0000	0.0000	0.0000	0.0000
1603.15	-22.3325	0.0000	0.0000	0.0000	0.0000	0.0000
1613.15	-23.4459	0.0000	0.0000	0.0000	0.0000	0.000

TABLE 4							
MOLAL THERMODYNAMIC FUNCTIONS FOR L-LEUCINE ((CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> (NH <sub>2</sub> )CHCOOH) SOLID PHASE							
GRAM MOLECULAR WT. = 131.17601 GRAMS T DEG K = 273.15 + T DEG C				1 CAL = 4.1840 JOULES			
T	C <sub>P</sub> <sup>C</sup>	(H <sub>T</sub> <sup>O</sup> -H <sub>0</sub> <sup>C</sup> )	(H <sub>T</sub> <sup>O</sup> -H <sub>0</sub> <sup>C</sup> )/T	S <sub>T</sub> <sup>O</sup>	-(C <sub>T</sub> <sup>O</sup> -H <sub>0</sub> <sup>C</sup> )	-(G <sub>T</sub> <sup>O</sup> -H <sub>0</sub> <sup>C</sup> )/T	
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG	
20.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000
50.00	0.169	0.086	0.017	0.023	0.029	0.006	0.006
100.00	0.535	1.360	0.136	0.182	0.458	0.046	
150.00	1.539	6.372	0.425	0.574	2.245	0.150	
200.00	2.752	17.072	0.854	1.182	6.562	0.328	
250.00	4.046	34.030	1.061	1.933	14.299	0.572	
300.00	5.390	57.616	1.020	2.799	26.064	0.867	
350.00	6.716	87.898	2.511	2.720	42.318	1.209	
400.00	7.968	124.464	3.116	4.700	62.352	1.584	
450.00	9.176	167.541	2.722	5.708	80.764	1.986	
500.00	10.337	216.321	4.327	6.736	120.47	2.409	
550.00	11.419	270.74	4.928	7.772	156.74	2.850	
600.00	12.474	330.48	5.508	8.811	196.19	3.303	
650.00	13.492	397.43	6.084	9.851	244.85	3.767	
700.00	14.448	465.82	6.647	10.886	296.62	4.235	
750.00	15.344	533.70	7.177	11.813	352.56	4.716	
800.00	16.217	601.84	7.705	12.834	415.81	5.198	
850.00	17.206	670.67	8.237	13.847	483.02	5.683	
900.00	18.149	740.82	8.787	14.857	558.29	6.170	
950.00	18.869	811.15	9.296	15.859	632.58	6.659	
1000.00	19.569	879.47	9.794	16.848	714.82	7.148	
1050.00	20.241	1079.6	10.282	17.820	801.98	7.638	
1100.00	21.167	1163.5	10.759	18.837	894.00	8.127	
1150.00	21.983	1291.2	11.226	19.844	990.82	8.616	
1200.00	22.619	1402.5	11.688	20.731	1092.4	9.104	
1250.00	23.224	1517.4	12.159	21.729	1198.7	9.590	
1300.00	24.019	1633.7	12.622	22.657	1302.7	10.075	
1350.00	24.861	1757.5	13.018	23.576	1425.3	10.558	
1400.00	25.956	1884.6	13.447	24.486	1545.4	11.039	
1450.00	26.220	2011.1	13.869	25.387	1670.1	11.518	
1500.00	26.476	2142.8	14.285	26.281	1799.1	11.995	
1550.00	27.319	2277.8	14.695	27.166	1932.9	12.470	
1600.00	27.940	2414.0	15.100	28.043	2070.3	12.943	
1650.00	28.608	2551.4	15.499	28.914	2213.3	13.414	
1700.00	29.261	2770.1	15.844	29.777	2360.1	13.882	
1750.00	29.430	2991.0	16.286	30.635	2511.1	14.349	
1800.00	30.544	3001.1	16.673	31.486	2666.4	14.813	
1850.00	31.160	3193.4	17.056	32.342	2820.0	15.275	
1900.00	31.767	3317.7	17.425	33.171	2981.7	15.735	
1950.00	32.370	3443.1	17.811	34.004	3157.7	16.193	
2000.00	32.904	3645.5	18.183	34.831	3327.7	16.649	
2050.00	33.644	3821.1	18.552	35.654	3506.0	17.102	
2100.00	34.246	3975.0	18.919	36.473	3685.3	17.554	
2150.00	34.797	4146.1	19.284	37.287	3870.7	18.003	
2200.00	35.608	4322.5	19.648	38.098	4059.1	18.451	
2250.00	36.273	4502.2	20.010	39.906	4251.7	18.866	
2300.00	36.847	4645.2	20.370	40.711	4448.2	19.260	
2350.00	37.423	4873.4	20.732	41.514	4644.8	19.782	
2400.00	38.401	5014.1	21.092	42.314	4852.3	20.222	
2450.00	39.147	5253.9	21.453	43.114	5061.9	20.661	
2500.00	39.858	5423.4	21.814	44.911	5274.5	21.098	
2550.00	40.608	5654.5	22.175	45.708	5491.0	21.532	
2600.00	41.344	5855.4	22.536	46.504	5711.5	21.967	
2650.00	42.157	6066.1	22.899	47.294	5936.0	22.400	
2700.00	42.943	6280.8	23.262	48.094	6164.5	22.832	
2750.00	43.647	6416.6	23.492	48.895	6310.5	23.103	
2800.00	44.340	6471.6	23.628	49.695	6397.0	23.262	
2850.00	44.944	6716.7	23.805	47.686	6633.4	23.691	
2900.00	45.577	6844.2	24.366	48.485	6873.0	24.119	
2950.00	46.156	7117.0	24.740	49.286	7116.3	24.546	
3000.00	46.747	7401.7	24.118	50.089	7366.7	24.972	
3050.00	48.147	7500.4	24.558	50.898	7525.0	25.240	
3100.00	48.506	7647.0	24.449	50.897	7614.2	25.397	

H<sub>0</sub><sup>C</sup> IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Hutchens, J. O., Cole, A. G. and Stout, J. W.,  
Heat capacities from 11 to 305 K., entropies, and free energies of formation  
of l-valine, l-isoleucine, and l-leucine,  
J. Phys. Chem. 67, 1128-1130 (1963).

TABLE 5

MOLAL THERMODYNAMIC FUNCTIONS FOR L-ISOLEUCINE  
 $((\text{CH}_3)_2\text{C}_2\text{H}_5\text{CH}(\text{NH}_2)\text{CHCOOH})$   
 SOLID PHASE

GRAM MOLECULAR WT. = 131.17601 GRAMS  
 $T \text{ DEG K} = 273.15 + T \text{ DEG C}$

1 CAL = 4.1840 JOULES

T DEG K	$C_p^c$ CAL/DEG	$(H_T^0 - H_0^c)$ CAL	$(H_T^0 - H_0^c)/T$ CAL/DEG	$S_T^o$ CAL/DEG	$-(G_T^0 - H_0^c)$ CAL	$-(G_T^0 - H_0^c)/T$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.045	0.104	0.022	0.024	0.037	0.007
10.00	0.047	0.102	0.014	0.015	0.057	0.006
15.00	0.044	0.101	0.011	0.013	0.056	0.011
20.00	0.044	0.101	0.011	0.013	0.056	0.011
25.00	0.044	0.101	0.011	0.013	0.056	0.011
30.00	0.044	0.101	0.011	0.013	0.056	0.011
35.00	0.044	0.101	0.011	0.013	0.056	0.011
40.00	0.044	0.101	0.011	0.013	0.056	0.011
45.00	0.044	0.101	0.011	0.013	0.056	0.011
50.00	0.044	0.101	0.011	0.013	0.056	0.011
55.00	0.044	0.101	0.011	0.013	0.056	0.011
60.00	0.044	0.101	0.011	0.013	0.056	0.011
65.00	0.044	0.101	0.011	0.013	0.056	0.011
70.00	0.044	0.101	0.011	0.013	0.056	0.011
75.00	0.044	0.101	0.011	0.013	0.056	0.011
80.00	0.044	0.101	0.011	0.013	0.056	0.011
85.00	0.044	0.101	0.011	0.013	0.056	0.011
90.00	0.044	0.101	0.011	0.013	0.056	0.011
95.00	0.044	0.101	0.011	0.013	0.056	0.011
100.00	0.044	0.101	0.011	0.013	0.056	0.011
105.00	0.044	0.101	0.011	0.013	0.056	0.011
110.00	0.044	0.101	0.011	0.013	0.056	0.011
115.00	0.044	0.101	0.011	0.013	0.056	0.011
120.00	0.044	0.101	0.011	0.013	0.056	0.011
125.00	0.044	0.101	0.011	0.013	0.056	0.011
130.00	0.044	0.101	0.011	0.013	0.056	0.011
135.00	0.044	0.101	0.011	0.013	0.056	0.011
140.00	0.044	0.101	0.011	0.013	0.056	0.011
145.00	0.044	0.101	0.011	0.013	0.056	0.011
150.00	0.044	0.101	0.011	0.013	0.056	0.011
155.00	0.044	0.101	0.011	0.013	0.056	0.011
160.00	0.044	0.101	0.011	0.013	0.056	0.011
165.00	0.044	0.101	0.011	0.013	0.056	0.011
170.00	0.044	0.101	0.011	0.013	0.056	0.011
175.00	0.044	0.101	0.011	0.013	0.056	0.011
180.00	0.044	0.101	0.011	0.013	0.056	0.011
185.00	0.044	0.101	0.011	0.013	0.056	0.011
190.00	0.044	0.101	0.011	0.013	0.056	0.011
195.00	0.044	0.101	0.011	0.013	0.056	0.011
200.00	0.044	0.101	0.011	0.013	0.056	0.011
205.00	0.044	0.101	0.011	0.013	0.056	0.011
210.00	0.044	0.101	0.011	0.013	0.056	0.011
215.00	0.044	0.101	0.011	0.013	0.056	0.011
220.00	0.044	0.101	0.011	0.013	0.056	0.011
225.00	0.044	0.101	0.011	0.013	0.056	0.011
230.00	0.044	0.101	0.011	0.013	0.056	0.011
235.00	0.044	0.101	0.011	0.013	0.056	0.011
240.00	0.044	0.101	0.011	0.013	0.056	0.011
245.00	0.044	0.101	0.011	0.013	0.056	0.011
250.00	0.044	0.101	0.011	0.013	0.056	0.011
255.00	0.044	0.101	0.011	0.013	0.056	0.011
260.00	0.044	0.101	0.011	0.013	0.056	0.011
265.00	0.044	0.101	0.011	0.013	0.056	0.011
270.00	0.044	0.101	0.011	0.013	0.056	0.011
275.00	0.044	0.101	0.011	0.013	0.056	0.011
280.00	0.044	0.101	0.011	0.013	0.056	0.011
285.00	0.044	0.101	0.011	0.013	0.056	0.011
290.00	0.044	0.101	0.011	0.013	0.056	0.011
295.00	0.044	0.101	0.011	0.013	0.056	0.011
300.00	0.044	0.101	0.011	0.013	0.056	0.011
305.00	0.044	0.101	0.011	0.013	0.056	0.011
310.00	0.044	0.101	0.011	0.013	0.056	0.011
315.00	0.044	0.101	0.011	0.013	0.056	0.011
320.00	0.044	0.101	0.011	0.013	0.056	0.011
325.00	0.044	0.101	0.011	0.013	0.056	0.011
330.00	0.044	0.101	0.011	0.013	0.056	0.011
335.00	0.044	0.101	0.011	0.013	0.056	0.011
340.00	0.044	0.101	0.011	0.013	0.056	0.011
345.00	0.044	0.101	0.011	0.013	0.056	0.011
350.00	0.044	0.101	0.011	0.013	0.056	0.011
355.00	0.044	0.101	0.011	0.013	0.056	0.011
360.00	0.044	0.101	0.011	0.013	0.056	0.011
365.00	0.044	0.101	0.011	0.013	0.056	0.011
370.00	0.044	0.101	0.011	0.013	0.056	0.011
375.00	0.044	0.101	0.011	0.013	0.056	0.011
380.00	0.044	0.101	0.011	0.013	0.056	0.011
385.00	0.044	0.101	0.011	0.013	0.056	0.011
390.00	0.044	0.101	0.011	0.013	0.056	0.011
395.00	0.044	0.101	0.011	0.013	0.056	0.011
400.00	0.044	0.101	0.011	0.013	0.056	0.011
405.00	0.044	0.101	0.011	0.013	0.056	0.011
410.00	0.044	0.101	0.011	0.013	0.056	0.011
415.00	0.044	0.101	0.011	0.013	0.056	0.011
420.00	0.044	0.101	0.011	0.013	0.056	0.011
425.00	0.044	0.101	0.011	0.013	0.056	0.011
430.00	0.044	0.101	0.011	0.013	0.056	0.011
435.00	0.044	0.101	0.011	0.013	0.056	0.011
440.00	0.044	0.101	0.011	0.013	0.056	0.011
445.00	0.044	0.101	0.011	0.013	0.056	0.011
450.00	0.044	0.101	0.011	0.013	0.056	0.011
455.00	0.044	0.101	0.011	0.013	0.056	0.011
460.00	0.044	0.101	0.011	0.013	0.056	0.011
465.00	0.044	0.101	0.011	0.013	0.056	0.011
470.00	0.044	0.101	0.011	0.013	0.056	0.011
475.00	0.044	0.101	0.011	0.013	0.056	0.011
480.00	0.044	0.101	0.011	0.013	0.056	0.011
485.00	0.044	0.101	0.011	0.013	0.056	0.011
490.00	0.044	0.101	0.011	0.013	0.056	0.011
495.00	0.044	0.101	0.011	0.013	0.056	0.011
500.00	0.044	0.101	0.011	0.013	0.056	0.011

$H_0^c$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Hutchens, J. O., Cole, A. G. and Stout, J. W.,  
 Heat capacities from 11 to 305°K., entropies, and free energies of formation  
 of l-valine, l-isoleucine, and l-leucine,  
 J. Phys. Chem. 67, 1128-1130 (1963).

TABLE 6

MOLAL THERMODYNAMIC FUNCTIONS FOR L-TYROSINE  
 $(HOCH_2CH_2(NH_2)CHCOOH)$   
 SOLID PHASE

GRAM MOLECULAR WT. = 161.19292 GRAMS T DEG K = 273.15 + T DEG C				1 CAL = 4.1840 JOULES		
T DEG K	C <sub>P</sub> CAL/DEG	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG	S <sub>T</sub> <sup>0</sup> CAL/DEG	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.035	0.044	0.009	0.012	0.015	0.003
10.00	0.079	0.097	0.070	0.093	0.232	0.023
15.00	0.113	0.1503	0.234	0.312	1.175	0.078
20.00	0.148	0.1336	0.517	0.699	3.634	0.182
25.00	0.182	0.1386	0.895	1.232	8.402	0.336
30.00	0.217	0.1655	1.355	1.894	16.166	0.539
35.00	0.252	0.1734	1.878	2.664	27.523	0.786
40.00	0.279	0.1732	2.443	3.517	42.948	1.074
45.00	0.313	0.1647	3.033	4.428	62.789	1.395
50.00	0.347	0.1818	3.636	5.382	87.299	1.746
55.00	0.380	0.2330	4.242	6.363	116.65	2.121
60.00	0.411	0.2905	4.842	7.358	150.95	2.516
65.00	0.441	0.3573	5.437	8.364	190.25	2.927
70.00	0.470	0.4214	6.021	9.373	234.59	3.351
75.00	0.499	0.4945	6.594	10.381	283.98	3.786
80.00	0.529	0.5725	7.157	11.387	338.40	4.230
85.00	0.559	0.6555	7.712	12.392	397.85	4.681
90.00	0.589	0.7430	8.257	13.393	462.51	5.137
95.00	0.616	0.8349	8.789	14.386	531.77	5.598
100.00	0.641	0.9307	9.307	15.369	606.16	6.062
105.00	0.661	1.0306	9.815	16.343	682.44	6.528
110.00	0.680	1.1347	10.315	17.311	769.58	6.996
115.00	0.705	1.2429	10.808	18.273	858.54	7.466
120.00	0.726	1.3552	11.293	19.229	952.30	7.936
125.00	0.746	1.4714	11.771	20.178	1050.8	8.407
130.00	0.764	1.5915	12.243	21.120	1154.1	8.877
135.00	0.784	1.7157	12.709	22.057	1264.0	9.348
140.00	0.804	1.8439	13.171	22.989	1374.6	9.819
145.00	0.821	1.9760	13.628	23.517	1491.9	10.289
150.00	0.839	2.1120	14.080	24.839	1613.8	10.759
155.00	0.859	2.2520	14.529	25.757	1740.3	11.228
160.00	0.876	2.3960	14.975	26.671	1871.4	11.696
165.00	0.892	2.5440	15.418	27.582	2007.0	12.164
170.00	0.904	2.6962	15.860	28.490	2147.2	12.630
175.00	0.918	2.8524	16.299	29.396	2291.9	13.096
180.00	0.931	3.0125	16.736	30.298	2441.1	13.562
185.00	0.932	3.1767	17.171	31.197	2594.9	14.026
190.00	0.937	3.3448	17.604	32.094	2753.1	14.490
195.00	0.941	3.5168	18.035	32.989	2915.8	14.953
200.00	0.942	3.6930	18.465	33.880	3083.0	15.415
205.00	0.944	3.8731	18.893	34.769	3254.6	15.876
210.00	0.946	4.0574	19.321	35.657	3430.7	16.336
215.00	0.948	4.2457	19.748	36.544	3611.2	16.796
220.00	0.949	4.4382	20.174	37.429	3796.1	17.255
225.00	0.951	4.6348	20.599	38.312	3985.4	17.713
230.00	0.952	4.8353	21.023	39.194	4179.2	18.170
235.00	0.953	5.0399	21.446	40.073	4377.4	18.627
240.00	0.953	5.2484	21.868	40.951	4579.9	19.083
245.00	0.951	5.4610	22.290	41.828	4786.9	19.538
250.00	0.947	5.6776	22.710	42.703	4998.2	19.993
255.00	0.945	5.8984	23.131	43.578	5213.9	20.447
260.00	0.941	6.1234	23.551	44.451	5434.0	20.900
265.00	0.938	6.3525	23.972	45.324	5658.4	21.353
270.00	0.930	6.5859	24.392	46.197	5887.2	21.805
275.00	0.924	6.7351	24.657	46.746	6033.6	22.089
280.00	0.914	6.8235	24.813	47.069	6120.4	22.256
285.00	0.902	7.0652	25.233	47.940	6357.9	22.707
290.00	0.891	7.3111	25.653	48.810	6599.8	23.157
295.00	0.879	7.5612	26.073	49.680	6846.0	23.607
298.15	0.875	7.8154	26.493	50.549	7096.6	24.056
300.00	0.878	7.9776	26.757	51.096	7256.7	24.339
		8074.7	26.912	51.417	7351.5	24.505

H<sub>0</sub><sup>C</sup> IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Huffman, H. M. and Ellis, E. L.,  
 Thermal data. VIII. The heat capacities, entropies and free energies of  
 some amino acids,  
 J. Am. Chem. Soc. 59, 2150-2152 (1937).

Cole, A. G., Hutchens, J. O., and Stout, J. W.,  
 Heat capacities from 11 to 305 K. and entropies of l-phenylalanine,  
 l-proline, l-tryptophane, and l-tyrosine. Some free energies of formation,  
 J. Phys. Chem. 67, 1852-1855 (1963).

TABLE 7

MOLAL THERMODYNAMIC FUNCTIONS FOR L-PHENYLALANINE  
 $(C_6H_5CH_2(NH_2)CHCOOH)$   
 SOLID PHASE

GRAM MOLECULAR WT. = 165.19352 GRAMS  
 T DEG K =  $273.15 + T$  DEG C      1 CAL = 4.1840 JOULES

T DEG K	$C_p^{\circ}$ CAL/DEG	$(H_T^0 - H_0^0)$ CAL	$(H_T^0 - H_0^0)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(C_T^0 - H_0^0)$ CAL	$-(C_T^0 - H_0^0)/T$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.074	0.093	0.019	0.025	0.031	0.006
10.00	0.157	1.469	0.147	0.196	0.493	0.049
15.00	1.597	6.745	0.450	0.610	2.406	0.160
20.00	2.836	17.774	0.889	1.236	6.948	0.347
25.00	4.157	35.240	1.410	2.010	19.013	0.601
30.00	5.534	59.442	1.981	2.889	27.222	0.907
35.00	6.915	90.591	2.588	3.846	44.033	1.258
40.00	8.211	128.44	3.211	4.855	65.771	1.644
45.00	9.426	172.57	3.835	5.893	92.634	2.059
50.00	10.567	222.57	4.451	6.946	124.73	2.495
55.00	11.652	278.15	5.057	8.005	162.10	2.947
60.00	12.667	338.26	5.649	9.062	204.77	3.413
65.00	13.617	404.67	6.226	10.114	252.72	3.888
70.00	14.511	475.03	6.786	11.156	305.90	4.370
75.00	15.366	549.73	7.330	12.186	364.26	4.857
80.00	16.251	628.78	7.866	13.206	427.74	5.347
85.00	17.083	712.14	8.378	14.217	496.31	5.839
90.00	17.852	799.49	8.883	15.215	564.89	6.332
95.00	18.588	890.60	9.375	16.200	648.44	6.826
100.00	19.314	985.36	9.854	17.172	731.87	7.319
105.00	20.050	1083.8	10.322	18.132	820.14	7.811
110.00	20.778	1185.8	10.780	19.082	913.18	8.302
115.00	21.486	1291.5	11.231	20.021	1010.9	8.791
120.00	22.163	1400.7	11.672	20.950	1113.4	9.278
125.00	22.844	1513.2	12.105	21.869	1220.4	9.763
130.00	23.544	1629.1	12.532	22.778	1332.1	10.247
135.00	24.256	1748.6	12.953	23.680	1448.2	10.727
140.00	24.949	1871.7	13.369	24.575	1568.8	11.206
145.00	25.627	1998.1	13.760	25.462	1693.9	11.682
150.00	26.319	2128.0	14.186	26.343	1823.5	12.156
155.00	27.031	2261.3	14.589	27.217	1957.4	12.628
160.00	27.746	2398.3	14.989	28.087	2095.6	13.098
165.00	28.455	2538.8	15.387	28.952	2236.2	13.565
170.00	29.164	2682.8	15.781	29.812	2385.1	14.030
175.00	29.872	2830.4	16.174	30.667	2536.3	14.493
180.00	30.579	2981.6	16.564	31.519	2691.8	14.954
185.00	31.287	3136.2	16.953	32.366	2851.5	15.414
190.00	31.999	3294.4	17.339	33.210	3015.4	15.871
195.00	32.714	3456.2	17.724	34.050	3183.6	16.326
200.00	33.427	3621.6	18.108	34.888	3355.9	16.780
205.00	34.141	3790.5	18.490	35.722	3532.5	17.232
210.00	34.861	3963.0	18.871	36.553	3713.2	17.682
215.00	35.597	4139.1	19.252	37.382	3898.0	18.130
220.00	36.349	4319.0	19.632	38.209	4087.0	18.577
225.00	37.116	4502.6	20.012	39.034	4280.1	19.023
230.00	37.888	4690.1	20.392	39.859	4477.3	19.467
235.00	38.662	4881.5	20.772	40.682	4678.7	19.909
240.00	39.435	5076.8	21.153	41.504	4884.1	20.351
245.00	40.206	5275.9	21.534	42.325	5093.7	20.791
250.00	40.279	5478.8	21.915	43.145	5307.4	21.229
255.00	41.755	5685.7	22.297	43.964	5525.1	21.667
260.00	42.556	5896.4	22.678	44.782	5747.0	22.104
265.00	43.320	6111.0	23.060	45.600	5973.0	22.539
270.00	44.106	6329.6	23.443	46.417	6203.0	22.974
273.15	44.600	6469.3	23.684	46.931	6350.0	23.247
275.00	44.890	6552.1	23.826	47.234	6437.1	23.408
280.00	45.671	6778.5	24.209	48.049	6675.3	23.841
285.00	46.448	7008.8	24.592	48.865	6917.6	24.272
290.00	47.221	7242.9	24.976	49.679	7164.0	24.703
295.00	47.993	7481.0	25.359	50.493	7414.4	25.134
298.15	48.481	7632.9	25.601	51.005	7574.3	25.404
300.00	48.768	7722.9	25.743	51.306	7668.9	25.563

$H_0^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Cole, A. G., Hutchens, J. O. and Stout, J. W.,  
 Heat capacities from 11 to 305 K. and entropies of L-phenylalanine,  
 L-proline, L-tryptophane, and L-tyrosine. Some free energies of formation,  
 J. Phys. Chem. 67, 1852-1855 (1963).

TABLE 8

MOLAL THERMODYNAMIC FUNCTIONS FOR L-TRYPTOPHANE  
 $(C_8H_6NCH_2(NH_2)CHCOOH)$   
SOLID PHASE

GRAM MOLECULAR WT. = 204.23049 GRAMS      1 CAL = 4.1840 JOULES  
T DEG K = 273.15 + T DEG C

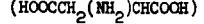
T DEG K	$C_p^C$	$(H_T^0 - H_0^C)$	$(H_T^0 - H_0^C)/T$	$S_T^0$	$-(G_T^0 - H_0^C)$	$-(G_T^0 - H_0^C)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.116	0.144	0.029	0.038	0.048	0.010
10.00	0.896	2.293	0.229	0.306	0.770	0.077
15.00	2.393	10.371	0.691	0.941	3.740	0.249
20.00	3.947	26.248	1.312	1.843	10.622	0.531
25.00	5.495	49.850	1.994	2.890	22.410	0.896
30.00	6.995	81.102	2.703	4.026	39.673	1.322
35.00	8.434	119.72	3.420	5.213	62.755	1.793
40.00	9.742	165.21	4.130	6.426	91.849	2.296
45.00	10.991	217.04	4.823	7.646	127.03	2.823
50.00	12.200	275.06	5.501	8.867	168.31	3.366
55.00	13.310	338.86	6.161	10.083	215.69	3.922
60.00	14.402	408.14	6.802	11.288	269.12	4.485
65.00	15.459	482.82	7.428	12.483	328.55	5.055
70.00	16.429	562.57	8.037	13.664	393.93	5.628
75.00	17.390	647.12	8.628	14.831	465.17	6.202
80.00	18.363	736.55	9.207	15.985	542.21	6.778
85.00	19.328	830.85	9.775	17.128	625.00	7.353
90.00	20.212	929.72	10.330	18.258	713.47	7.927
95.00	21.092	1033.0	10.873	19.374	807.55	8.501
100.00	21.972	1140.7	11.407	20.478	907.19	9.072
105.00	22.848	1252.7	11.931	21.572	1012.3	9.641
110.00	23.674	1369.0	12.445	22.652	1122.9	10.208
115.00	24.514	1489.5	12.952	23.724	1238.8	10.772
120.00	25.341	1614.1	13.451	24.785	1360.1	11.334
125.00	26.169	1742.9	13.943	25.836	1486.7	11.893
130.00	27.025	1875.8	14.430	26.879	1618.5	12.450
135.00	27.898	2013.2	14.912	27.916	1755.5	13.003
140.00	28.763	2154.8	15.392	28.946	1897.6	13.554
145.00	29.606	2300.7	15.867	29.970	2044.9	14.103
150.00	30.444	2450.9	16.339	30.988	2197.3	14.649
155.00	31.296	2605.2	16.808	32.000	2354.8	15.192
160.00	32.159	2763.8	17.274	33.007	2517.3	15.733
165.00	33.019	2926.8	17.738	34.010	2684.8	16.272
170.00	33.871	3094.0	18.200	35.008	2857.4	16.808
175.00	34.721	3265.5	18.660	36.002	3034.9	17.342
180.00	35.576	3441.2	19.118	36.992	3217.4	17.874
185.00	36.442	3621.3	19.575	37.979	3404.8	18.404
190.00	37.316	3805.7	20.030	38.962	3597.2	18.933
195.00	38.191	3994.4	20.484	39.943	3794.4	19.459
200.00	39.065	4187.6	20.938	40.921	3996.6	19.983
205.00	39.942	4385.1	21.391	41.896	4203.6	20.506
210.00	40.825	4587.0	21.843	42.869	4415.6	21.026
215.00	41.713	4793.4	22.295	43.840	4632.3	21.546
220.00	42.601	5004.1	22.746	44.810	4854.0	22.063
225.00	43.489	5219.4	23.197	45.777	5080.4	22.580
230.00	44.383	5439.0	23.648	46.742	5311.7	23.094
235.00	45.287	5663.2	24.099	47.707	5547.9	23.608
240.00	46.200	5891.9	24.550	48.670	5788.8	24.120
245.00	47.120	6125.2	25.001	49.632	6034.5	24.631
250.00	48.042	6363.1	25.453	50.593	6285.1	25.140
255.00	48.964	6605.6	25.904	51.553	6540.5	25.649
260.00	49.884	6852.8	26.357	52.513	6800.6	26.156
265.00	50.800	7104.5	26.809	53.472	7065.6	26.663
270.00	51.712	7360.8	27.262	54.430	7335.4	27.168
275.00	52.625	7524.6	27.547	55.033	7507.8	27.486
280.00	53.540	7621.6	27.715	55.387	7609.9	27.672
285.00	54.468	7887.0	28.168	56.344	7889.2	28.176
290.00	55.409	8157.0	28.621	57.299	8173.3	28.678
295.00	56.360	8431.7	29.075	58.255	8462.2	29.180
298.15	56.958	8889.6	29.529	59.210	8755.9	29.681
300.00	57.307	8990.4	29.954	59.812	8943.3	29.996
				60.165	9054.3	30.181

$H_0^C$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Cole, A. G., Hutchens, J. O. and Stout, J. W.,  
Heat capacities from 11 to 305 K. and entropies of L-phenylalanine,  
L-proline, L-tryptophane, and L-tyrosine. Some free energies of formation,  
J. Phys. Chem. 67, 1852-1855 (1963).

TABLE 9

## MOLAL THERMODYNAMIC FUNCTIONS FOR L-ASPARTIC ACID



SOLID PHASE

GRAM MOLECULAR WT. = 133.10469 GRAMS  
T DEG K = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

T DEG K	$C_p^C$ CAL/DEG	$(H_T^0 - H_0^C)$ CAL	$(H_T^0 - H_0^C)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(Q_T^0 - H_0^C)$ CAL	$-(Q_T^0 - H_0^C)/T$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.022	0.022	0.005	0.007	0.000	0.002
10.00	0.101	0.143	0.044	0.050	0.146	0.015
15.00	0.199	0.234	0.056	0.066	0.177	0.050
20.00	0.444	0.444	0.031	0.093	0.444	0.122
25.00	0.467	0.151	0.065	0.922	0.928	0.237
30.00	0.619	0.100	0.077	1.473	11.870	0.396
35.00	0.823	0.046	0.026	2.121	20.818	0.595
40.00	0.817	0.016	0.013	2.843	33.200	0.830
45.00	7.184	113.53	2.523	3.619	49.336	1.096
50.00	8.294	152.76	3.043	4.434	69.457	1.389
55.00	9.340	196.36	3.570	5.274	93.720	1.704
60.00	10.343	245.54	4.093	6.130	122.23	2.037
65.00	11.288	299.04	4.611	6.490	155.04	2.385
70.00	12.154	358.34	5.117	7.865	192.19	2.746
75.00	12.962	421.17	5.616	8.142	233.68	3.116
80.00	13.796	488.14	6.142	9.500	279.00	3.494
85.00	14.673	554.10	6.670	10.456	320.63	3.875
90.00	15.287	633.61	7.042	11.310	384.05	4.267
95.00	15.939	711.97	7.494	12.155	442.71	4.660
100.00	16.601	793.38	7.934	12.990	505.58	5.056
105.00	17.222	877.94	8.361	13.813	572.59	5.453
110.00	17.857	965.78	8.776	14.630	643.71	5.852
115.00	18.442	1056.62	9.183	15.426	718.87	6.251
120.00	19.011	1149.7	9.592	16.233	798.05	6.650
125.00	19.577	1246.0	10.010	17.020	861.18	7.045
130.00	20.124	1345.0	10.430	17.798	968.23	7.448
135.00	20.687	1447.6	10.723	18.568	1059.2	7.846
140.00	21.219	1552.3	11.088	19.330	1153.9	8.242
145.00	21.747	1659.0	11.447	20.084	1252.4	8.636
150.00	22.273	1769.8	11.799	20.830	1354.7	9.032
155.00	22.795	1862.5	12.145	21.559	1460.7	9.424
160.00	23.321	1997.8	12.496	22.301	1570.4	9.815
165.00	23.842	2115.7	12.822	23.027	1683.7	10.204
170.00	24.360	2236.2	13.154	23.746	1800.7	10.592
175.00	24.841	2355.2	13.481	24.459	1921.2	10.978
180.00	25.334	2484.5	13.804	25.166	2045.3	11.363
185.00	25.854	2612.8	14.122	25.867	2172.5	11.745
190.00	26.378	2740.2	14.438	26.564	2303.6	12.126
195.00	26.864	2870.4	14.751	27.266	2438.9	12.505
200.00	27.351	3012.0	15.060	27.967	2576.0	12.882
205.00	27.823	3147.7	15.366	28.624	2717.3	13.258
210.00	28.291	3290.2	15.668	29.300	2862.7	13.632
215.00	28.772	3432.4	16.967	29.971	3010.9	14.004
220.00	29.260	3570.0	16.263	30.638	3162.4	14.375
225.00	29.754	3727.5	16.558	31.301	3317.2	14.743
230.00	30.262	3875.0	16.857	31.961	3475.4	15.110
235.00	30.751	4026.8	17.141	32.617	3636.8	15.476
240.00	31.264	4183.2	17.430	33.270	3801.6	15.840
245.00	31.767	4240.0	17.718	33.920	3969.0	16.204
250.00	32.219	4300.9	18.003	34.566	4140.8	16.563
255.00	32.755	4363.4	18.288	35.210	4315.2	16.922
260.00	33.248	4426.4	18.571	35.851	4492.9	17.280
265.00	33.741	4495.9	18.852	36.489	4673.7	17.637
270.00	34.243	5165.8	19.133	37.124	4857.7	17.992
275.00	34.743	5274.1	19.309	37.523	4975.3	18.215
280.00	34.725	5338.2	19.412	37.757	5044.9	18.345
285.00	35.223	5513.1	19.690	38.387	5235.3	18.698
290.00	35.730	5697.4	19.966	39.015	5428.8	19.048
295.00	36.248	5870.4	20.243	39.641	5625.4	19.398
298.15	36.775	6052.9	20.518	40.265	5825.2	19.746
300.00	37.304	6238.1	20.794	40.887	6028.1	20.094

 $H_0^C$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Huffman, H. M. and Borsook, H.,  
 Thermal data. I. The heat capacities, entropies and free energies of  
 seven organic compounds containing nitrogen,  
*J. Am. Chem. Soc.* 54, 4297-4301 (1932).

Hutchens, J. O., Cole, A. G., Robbie, R. A. and Stout, J. W.,  
 Heat capacities from 11 to 305°K, entropies and free energies of formation  
 of l-asparagine monohydrate, l-aspartic acid, l-glutamic acid, and l-glutamine,  
*J. Biol. Chem.* 238, 2407-2412 (1963).

TABLE 10

MOLAL THERMODYNAMIC FUNCTIONS FOR L-ASPARAGINE MONOHYDRATE  
 $(\text{NH}_2\text{COCH}_2(\text{NH}_2)\text{CHCOOH}\cdot\text{H}_2\text{O})$   
 SOLID PHASE

GRAM MOLECULAR WT. = 150.13530 GRAMS  
 T DEG K = 273.15 + T DEG C      1 CAL = 4,1840 JOULES

T DEG K	$C_p^C$ CAL/DEG	$(H_{T=0}^0 - H_0^0)$ CAL	$(H_{T=0}^0 - H_0^0)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(G_{T=0}^0 - G_0^0)$ CAL	$-(G_{T=0}^0 - G_0^0)/T$ CAL/DEG
273.15	0.370	0.000	0.000	0.000	0.000	0.000
274.00	0.370	0.005	0.005	0.007	0.008	0.002
275.00	0.364	0.402	0.041	0.054	0.135	0.014
276.00	0.362	0.403	0.140	0.186	0.692	0.046
277.00	0.354	0.580	0.329	0.439	2.197	0.110
278.00	0.279	15.267	0.619	0.626	3.307	0.212
279.00	0.247	29.745	0.691	1.348	10.642	0.356
280.00	0.200	50.573	1.445	1.987	16.985	0.542
281.00	0.258	76.331	1.958	2.727	30.732	0.768
282.00	0.278	114.17	2.515	3.546	46.353	1.031
283.00	0.272	150.07	3.101	4.427	66.422	1.326
284.00	0.260	174.77	3.705	5.255	90.722	1.650
285.00	0.255	223.03	4.317	6.315	112.84	1.998
286.00	0.246	320.69	4.833	7.302	113.92	2.348
287.00	0.231	384.32	5.547	8.304	192.94	2.756
288.00	0.217	451.51	6.153	9.313	225.98	3.160
289.00	0.204	510.13	6.752	10.328	285.04	3.576
290.00	0.192	524.20	7.342	11.345	340.26	4.003
291.00	0.187	713.13	7.924	12.363	337.53	4.434
292.00	0.185	800.83	8.493	13.376	465.88	4.883
293.00	0.186	894.93	9.049	14.382	133.24	5.323
294.00	0.187	1000.4	9.594	15.382	607.60	5.798
295.00	0.197	1114.2	10.129	16.375	657.04	6.246
296.00	0.218	1227.2	10.654	17.362	711.43	6.708
297.00	0.240	1247.4	11.170	18.343	860.70	7.172
298.00	0.245	1432.7	11.678	19.316	954.85	7.639
299.00	0.219	1551.0	12.177	20.283	1053.8	8.107
300.00	0.216	1710.4	12.669	21.244	1157.7	8.575
301.00	0.204	1841.6	13.154	22.199	1266.3	9.045
302.00	0.214	1976.7	13.633	23.147	1379.6	9.515
303.00	0.217	2117.7	14.105	24.030	1497.7	9.969
304.00	0.213	2228.6	14.572	25.027	1620.0	10.455
305.00	0.214	2403.3	15.035	25.958	1748.0	10.925
306.00	0.215	2439.7	15.489	26.884	1880.1	11.395
307.00	0.212	2711.0	15.941	27.805	2016.8	11.864
308.00	0.214	2861.0	16.388	28.721	2158.1	12.332
309.00	0.217	3020.8	16.832	29.632	2304.0	12.800
310.00	0.216	3195.3	17.272	30.539	2454.5	13.267
311.00	0.217	3264.6	17.708	31.442	2609.4	13.734
312.00	0.214	3347.4	18.140	32.340	2768.9	14.199
313.00	0.215	3715.6	18.569	33.233	2932.8	14.664
314.00	0.217	3891.0	18.994	34.122	3101.2	15.128
315.00	0.217	4071.4	19.416	35.007	3274.0	15.591
316.00	0.216	4261.6	19.835	35.888	3451.3	16.052
317.00	0.217	4455.4	20.252	36.765	3632.9	16.513
318.00	0.211	4547.9	20.666	37.639	3818.9	16.973
319.00	0.217	4847.6	21.078	38.510	4009.3	17.432
320.00	0.212	5047.6	21.488	39.377	4204.0	17.889
321.00	0.212	5244.9	21.896	40.242	4402.0	18.346
322.00	0.213	5461.9	22.302	41.103	4606.4	18.802
323.00	0.214	5676.5	22.706	41.962	4814.1	19.256
324.00	0.216	5892.7	23.109	42.819	5026.0	19.710
325.00	0.212	6112.6	23.510	43.672	5242.3	20.163
326.00	0.212	6330.0	23.909	44.523	5452.7	20.614
327.00	0.213	6562.9	24.307	45.372	5687.5	21.065
328.00	0.213	6797.6	24.557	45.905	5831.2	21.348
329.00	0.214	6794.3	24.703	46.217	5918.5	21.514
330.00	0.215	7027.3	25.097	47.061	6149.6	21.963
331.00	0.216	7264.8	25.491	47.901	6387.1	22.411
332.00	0.216	7506.0	25.883	48.740	6628.7	22.857
333.00	0.213	7750.7	26.274	49.577	6874.5	23.303
334.00	0.213	7906.8	26.519	50.103	7031.4	23.584
335.00	0.214	7994.1	26.664	50.412	7124.4	23.748

$H_0^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Huffman, H. M. and Borsook, H.,  
 Thermal data. I. The heat capacities, entropies and free energies of  
 seven organic compounds containing nitrogen,  
*J. Am. Chem. Soc.* 54, 4297-4301 (1932).

Hutchens, J. O., Cole, A. G., Robie, R. A. and Stout, J. W.,  
 Heat capacities from 11 to 305°K, entropies and free energies of formation  
 of l-asparagine monohydrate, l-aspartic acid, l-glutamic acid, and l-glutamine,  
*J. Biol. Chem.* 238, 2407-2412 (1963).

TABLE II

MOLAL THERMODYNAMIC FUNCTIONS FOR L-GLUTAMIC ACID  
 $(HOOC(CH_2)_2(NH_2)CHCOOH)$   
 SOLID PHASE

GRAM MOLECULAR WT. = 147.13178 GRAMS  
 T DEG K = 273.15 + T DEG C

1 CAL = 4,1840 JOULES

T DEG K	C <sub>P</sub> CAL/DEG	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG	S <sub>T</sub> <sup>0</sup> CAL/DEG	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.001	0.000	0.000	0.001	0.002
10.00	0.002	0.002	0.000	0.000	0.002	0.001
15.00	0.005	0.005	0.000	0.000	0.007	0.001
20.00	0.009	0.009	0.000	0.000	0.014	0.001
25.00	0.014	0.014	0.000	0.000	0.024	0.001
30.00	0.019	0.019	0.000	0.000	0.036	0.001
35.00	0.024	0.024	0.000	0.000	0.050	0.001
40.00	0.029	0.029	0.000	0.000	0.064	0.001
45.00	0.034	0.034	0.000	0.000	0.078	0.001
50.00	0.039	0.039	0.000	0.000	0.092	0.001
55.00	0.044	0.044	0.000	0.000	0.106	0.001
60.00	0.049	0.049	0.000	0.000	0.120	0.001
65.00	0.054	0.054	0.000	0.000	0.134	0.001
70.00	0.059	0.059	0.000	0.000	0.148	0.001
75.00	0.064	0.064	0.000	0.000	0.162	0.001
80.00	0.069	0.069	0.000	0.000	0.176	0.001
85.00	0.074	0.074	0.000	0.000	0.190	0.001
90.00	0.079	0.079	0.000	0.000	0.204	0.001
95.00	0.084	0.084	0.000	0.000	0.218	0.001
100.00	0.089	0.089	0.000	0.000	0.232	0.001
105.00	0.094	0.094	0.000	0.000	0.246	0.001
110.00	0.100	0.100	0.000	0.000	0.260	0.001
115.00	0.105	0.105	0.000	0.000	0.274	0.001
120.00	0.110	0.110	0.000	0.000	0.288	0.001
125.00	0.115	0.115	0.000	0.000	0.302	0.001
130.00	0.120	0.120	0.000	0.000	0.316	0.001
135.00	0.125	0.125	0.000	0.000	0.330	0.001
140.00	0.130	0.130	0.000	0.000	0.344	0.001
145.00	0.135	0.135	0.000	0.000	0.358	0.001
150.00	0.140	0.140	0.000	0.000	0.372	0.001
155.00	0.145	0.145	0.000	0.000	0.386	0.001
160.00	0.150	0.150	0.000	0.000	0.400	0.001
165.00	0.155	0.155	0.000	0.000	0.414	0.001
170.00	0.160	0.160	0.000	0.000	0.428	0.001
175.00	0.165	0.165	0.000	0.000	0.442	0.001
180.00	0.170	0.170	0.000	0.000	0.456	0.001
185.00	0.175	0.175	0.000	0.000	0.470	0.001
190.00	0.180	0.180	0.000	0.000	0.484	0.001
195.00	0.185	0.185	0.000	0.000	0.498	0.001
200.00	0.190	0.190	0.000	0.000	0.512	0.001
205.00	0.195	0.195	0.000	0.000	0.526	0.001
210.00	0.200	0.200	0.000	0.000	0.540	0.001
215.00	0.205	0.205	0.000	0.000	0.554	0.001
220.00	0.210	0.210	0.000	0.000	0.568	0.001
225.00	0.215	0.215	0.000	0.000	0.582	0.001
230.00	0.220	0.220	0.000	0.000	0.596	0.001
235.00	0.225	0.225	0.000	0.000	0.610	0.001
240.00	0.230	0.230	0.000	0.000	0.624	0.001
245.00	0.235	0.235	0.000	0.000	0.638	0.001
250.00	0.240	0.240	0.000	0.000	0.652	0.001
255.00	0.245	0.245	0.000	0.000	0.666	0.001
260.00	0.250	0.250	0.000	0.000	0.680	0.001
265.00	0.255	0.255	0.000	0.000	0.694	0.001
270.00	0.260	0.260	0.000	0.000	0.708	0.001
275.00	0.265	0.265	0.000	0.000	0.722	0.001
280.00	0.270	0.270	0.000	0.000	0.736	0.001
285.00	0.275	0.275	0.000	0.000	0.750	0.001
290.00	0.280	0.280	0.000	0.000	0.764	0.001
295.00	0.285	0.285	0.000	0.000	0.778	0.001
300.00	0.290	0.290	0.000	0.000	0.792	0.001
305.00	0.295	0.295	0.000	0.000	0.806	0.001
310.00	0.300	0.300	0.000	0.000	0.820	0.001
315.00	0.305	0.305	0.000	0.000	0.834	0.001
320.00	0.310	0.310	0.000	0.000	0.848	0.001
325.00	0.315	0.315	0.000	0.000	0.862	0.001
330.00	0.320	0.320	0.000	0.000	0.876	0.001
335.00	0.325	0.325	0.000	0.000	0.890	0.001
340.00	0.330	0.330	0.000	0.000	0.904	0.001
345.00	0.335	0.335	0.000	0.000	0.918	0.001
350.00	0.340	0.340	0.000	0.000	0.932	0.001
355.00	0.345	0.345	0.000	0.000	0.946	0.001
360.00	0.350	0.350	0.000	0.000	0.960	0.001
365.00	0.355	0.355	0.000	0.000	0.974	0.001
370.00	0.360	0.360	0.000	0.000	0.988	0.001
375.00	0.365	0.365	0.000	0.000	1.002	0.001
380.00	0.370	0.370	0.000	0.000	1.016	0.001
385.00	0.375	0.375	0.000	0.000	1.030	0.001
390.00	0.380	0.380	0.000	0.000	1.044	0.001
395.00	0.385	0.385	0.000	0.000	1.058	0.001
400.00	0.390	0.390	0.000	0.000	1.072	0.001
405.00	0.395	0.395	0.000	0.000	1.086	0.001
410.00	0.400	0.400	0.000	0.000	1.100	0.001
415.00	0.405	0.405	0.000	0.000	1.114	0.001
420.00	0.410	0.410	0.000	0.000	1.128	0.001
425.00	0.415	0.415	0.000	0.000	1.142	0.001
430.00	0.420	0.420	0.000	0.000	1.156	0.001
435.00	0.425	0.425	0.000	0.000	1.170	0.001
440.00	0.430	0.430	0.000	0.000	1.184	0.001
445.00	0.435	0.435	0.000	0.000	1.198	0.001
450.00	0.440	0.440	0.000	0.000	1.212	0.001
455.00	0.445	0.445	0.000	0.000	1.226	0.001
460.00	0.450	0.450	0.000	0.000	1.240	0.001
465.00	0.455	0.455	0.000	0.000	1.254	0.001
470.00	0.460	0.460	0.000	0.000	1.268	0.001
475.00	0.465	0.465	0.000	0.000	1.282	0.001
480.00	0.470	0.470	0.000	0.000	1.296	0.001
485.00	0.475	0.475	0.000	0.000	1.310	0.001
490.00	0.480	0.480	0.000	0.000	1.324	0.001
495.00	0.485	0.485	0.000	0.000	1.338	0.001
500.00	0.490	0.490	0.000	0.000	1.352	0.001
505.00	0.495	0.495	0.000	0.000	1.366	0.001
510.00	0.500	0.500	0.000	0.000	1.380	0.001
515.00	0.505	0.505	0.000	0.000	1.394	0.001
520.00	0.510	0.510	0.000	0.000	1.408	0.001
525.00	0.515	0.515	0.000	0.000	1.422	0.001
530.00	0.520	0.520	0.000	0.000	1.436	0.001
535.00	0.525	0.525	0.000	0.000	1.450	0.001
540.00	0.530	0.530	0.000	0.000	1.464	0.001
545.00	0.535	0.535	0.000	0.000	1.478	0.001
550.00	0.540	0.540	0.000	0.000	1.492	0.001
555.00	0.545	0.545	0.000	0.000	1.506	0.001
560.00	0.550	0.550	0.000	0.000	1.520	0.001
565.00	0.555	0.555	0.000	0.000	1.534	0.001
570.00	0.560	0.560	0.000	0.000	1.548	0.001
575.00	0.565	0.565	0.000	0.000	1.562	0.001
580.00	0.570	0.570	0.000	0.000	1.576	0.001
585.00	0.575	0.575	0.000	0.000	1.590	0.001
590.00	0.580	0.580	0.000	0.000	1.604	0.001
595.00	0.585	0.585	0.000	0.000	1.618	0.001
600.00	0.590	0.590	0.000	0.000	1.632	0.001
605.00	0.595	0.595	0.000	0.000	1.646	0.001
610.00	0.600	0.600	0.000	0.000	1.660	0.001
615.00	0.605	0.605	0.000	0.000	1.674	0.001
620.00	0.610	0.610	0.000	0.000	1.688	0.001
625.00	0.615	0.615	0.000	0.000	1.702	0.001
630.00	0.620	0.620	0.000	0.000	1.716	0.001
635.00	0.625	0.625	0.000	0.000	1.730	0.001
640.00	0.630	0.630	0.000	0.000	1.744	0.001
645.00	0.635	0.635	0.000	0.000	1.758	0.001
650.00	0.640	0.640	0.000	0.000	1.772	0.001
655.00	0.645	0.645	0.000	0.000	1.786	0.001
660.00	0.650	0.650	0.000	0.000	1.800	0.001
665.00	0.655	0.655	0.000	0.000	1.814	0.001
670.00	0.660	0.660	0.000	0.000	1.828	0.001
675.00	0.665	0.665	0.000	0.000	1.842	0.001
680.00	0.670	0.670	0.000	0.000	1.856	0.001
685.00	0.675	0.675	0.000	0.000	1.870	0.001
690.00	0.680	0.680	0.000	0.000	1.884	0.001
695.00	0.685	0.685	0.000	0.000	1.898	0.001
700.00	0.690	0.690	0.000	0.000	1.912	0.001
705.00	0.695	0.695	0.000	0.000	1.926	0.001
710.00	0.700	0.700	0.000	0.000	1.940	0.001
715.00	0.705	0.705	0.000	0.000	1.954	0.001
720.00	0.					

TABLE 12

MOLAL THERMODYNAMIC FUNCTIONS FOR L-GLUTAMINE  
 $(\text{NH}_2\text{CO}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH})$   
SOLID PHASE

GRAM MOLECULAR WT. = 146.14705 GRAMS

T DEG K = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

T DEG K	$C_p^C$ CAL/DEG	$(H_T^0 - H_0^C)$ CAL	$(H_T^0 - H_0^C)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(d_T^0 - H_0^C)$ CAL	$-(d_T^0 - H_0^C)/T$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.022	0.028	0.006	0.007	0.009	0.002
10.00	0.177	0.444	0.044	0.059	0.148	0.015
15.00	0.598	2.244	0.150	0.200	0.749	0.050
20.00	1.389	7.048	0.352	0.471	2.363	0.118
25.00	2.507	16.686	0.667	0.896	5.715	0.229
30.00	3.811	32.420	1.081	1.466	11.564	0.385
35.00	5.217	54.969	1.571	2.159	20.580	0.588
40.00	6.617	84.568	2.114	2.947	33.310	0.833
45.00	7.991	121.10	2.691	3.806	50.166	1.115
50.00	9.304	164.38	3.288	4.717	71.455	1.429
55.00	10.527	213.99	3.891	5.661	97.389	1.771
60.00	11.693	269.56	4.493	6.628	128.10	2.135
65.00	12.771	330.77	5.089	7.607	163.69	2.518
70.00	13.760	397.13	5.673	8.590	204.18	2.917
75.00	14.695	468.28	6.244	9.572	249.59	3.328
80.00	15.615	544.05	6.801	10.549	299.89	3.749
85.00	16.554	624.49	7.347	11.524	355.08	4.177
90.00	17.391	709.40	7.882	12.495	415.13	4.613
95.00	18.125	798.21	8.402	13.455	480.00	5.053
100.00	18.863	890.58	8.907	14.403	549.65	5.497
105.00	19.593	986.82	9.398	15.341	624.02	5.943
110.00	20.316	1086.6	9.878	16.270	703.05	6.391
115.00	21.031	1190.0	10.348	17.189	786.70	6.841
120.00	21.691	1296.8	10.807	18.098	874.92	7.291
125.00	22.323	1406.8	11.255	18.996	967.66	7.741
130.00	22.991	1520.1	11.693	19.884	1064.9	8.191
135.00	23.678	1636.8	12.124	20.765	1166.5	8.641
140.00	24.339	1756.8	12.549	21.638	1272.5	9.089
145.00	24.977	1880.1	12.966	22.503	1382.9	9.537
150.00	25.615	2006.6	13.377	23.361	1497.5	9.983
155.00	26.259	2136.3	13.783	24.211	1616.5	10.429
160.00	26.903	2269.2	14.182	25.055	1739.6	10.873
165.00	27.546	2405.3	14.578	25.893	1867.0	11.315
170.00	28.183	2544.6	14.969	26.725	1998.5	11.756
175.00	28.815	2687.1	15.355	27.551	2134.2	12.196
180.00	29.440	2832.8	15.738	28.371	2274.0	12.634
185.00	30.061	2981.5	16.116	29.186	2417.9	13.070
190.00	30.679	3133.4	16.491	29.996	2565.9	13.505
195.00	31.296	3288.3	16.863	30.801	2717.9	13.938
200.00	31.916	3446.4	17.232	31.601	2873.9	14.369
205.00	32.539	3607.5	17.597	32.397	3033.9	14.799
210.00	33.163	3771.7	17.961	33.189	3197.9	15.228
215.00	33.787	3939.1	18.321	33.976	3365.8	15.655
220.00	34.413	4109.6	18.680	34.760	3537.6	16.080
225.00	35.049	4283.3	19.037	35.541	3713.4	16.504
230.00	35.696	4460.1	19.392	36.318	3893.0	16.926
235.00	36.351	4640.2	19.746	37.093	4076.5	17.347
240.00	37.007	4823.6	20.098	37.865	4263.9	17.766
245.00	37.654	5010.3	20.450	38.635	4455.2	18.184
250.00	38.285	5200.1	20.801	39.402	4650.3	18.601
255.00	38.897	5393.1	21.149	40.166	4849.2	19.016
260.00	39.492	5589.1	21.497	40.927	5051.9	19.431
265.00	40.075	5780.0	21.842	41.685	5258.5	19.843
270.00	40.655	5989.8	22.185	42.439	5468.8	20.255
275.00	41.021	6118.5	22.400	42.913	5603.2	20.513
280.00	41.237	6194.6	22.526	43.191	5682.9	20.665
285.00	42.408	6612.8	23.203	44.684	6122.2	21.482
290.00	42.987	6826.3	23.539	45.427	6347.5	21.888
295.00	43.563	7042.7	23.873	46.167	6576.5	22.293
298.15	43.827	7180.4	24.083	46.631	6722.7	22.548
300.00	44.144	7261.1	24.216	46.904	6800.2	22.697

 $H_0^C$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Hutchens, J. O., Cone, A. G., Robie, R. A. and Stout, J. W.,  
Heat capacities from 11 to 305°K, entropies and free energies of formation  
of l-asparagine monohydrate, l-aspartic acid, l-glutamic acid, and l-glutamine,  
J. Biol. Chem. 238, 2407-2412 (1963).

TABLE 13

MOLAL THERMODYNAMIC FUNCTIONS FOR L-LYSINE HYDROCHLORIDE  
 $((\text{NH}_3^+ \text{Cl})(\text{CH}_2)_4(\text{NH}_2)\text{CHCOOH})$   
 SOLID PHASE

GRAM MOLECULAR WT. = 182.65165 GRAMS				1 CAL = 4,1840 JOULES		
T	$C_p^{\text{C}}$	$(H_{T=0}^0 - H_0^0)$	$(H_{T=0}^0 - H_0^0)/T$	$S_T^0$	$-(G_T^0 - G_0^0)$	$-(G_T^0 - G_0^0)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.062	0.077	0.015	0.021	0.026	0.005
10.00	0.199	1.248	0.125	0.166	0.415	0.041
15.00	1.552	6.139	0.409	0.549	2.089	0.139
20.00	2.934	17.290	0.864	1.181	6.322	0.316
25.00	4.496	37.782	1.431	1.999	14.202	0.568
30.00	6.101	62.472	2.082	2.568	26.565	0.886
35.00	7.913	97.742	2.793	4.052	44.074	1.259
40.00	9.884	141.51	3.538	5.710	67.221	1.681
45.00	11.927	194.50	4.300	6.441	96.250	2.141
50.00	13.938	253.62	5.072	7.706	131.70	2.634
55.00	16.024	321.76	5.850	9.004	173.47	3.154
60.00	17.184	391.738	6.623	10.319	221.77	3.696
65.00	17.297	430.18	7.387	11.644	276.68	4.257
70.00	18.549	502.75	8.139	12.971	338.22	4.832
75.00	19.785	565.59	8.875	14.293	406.38	5.418
80.00	21.042	627.66	9.596	15.610	481.14	6.014
85.00	21.377	675.59	10.306	16.923	562.47	6.617
90.00	21.821	720.19	11.002	18.228	650.25	7.226
95.00	22.354	764.6	11.680	19.520	744.72	7.839
100.00	23.411	1234.1	12.341	20.797	847.53	8.455
105.00	24.332	1364.6	12.987	22.060	952.67	9.073
110.00	27.373	1498.1	13.619	23.511	1066.1	9.692
115.00	28.314	1637.3	14.238	24.548	1189.8	10.311
120.00	29.213	1781.1	14.843	25.773	1311.5	10.930
125.00	31.077	1924.4	15.435	26.582	1443.5	11.548
130.00	30.826	2081.5	16.015	28.177	1581.0	12.164
135.00	31.777	2239.7	16.583	29.562	1720.2	12.779
140.00	32.571	2397.6	17.140	30.532	1870.0	13.393
145.00	33.302	2564.7	17.686	31.600	2030.5	14.004
150.00	34.140	2731.2	18.223	32.835	2191.5	14.612
155.00	34.940	2896.3	18.750	33.962	2368.0	15.210
160.00	35.730	3064.0	19.269	35.001	2531.5	15.822
165.00	36.492	3229.6	19.779	36.202	2709.6	16.423
170.00	37.240	3448.0	20.282	37.303	2893.5	17.021
175.00	38.102	3636.1	20.778	38.394	3082.8	17.616
180.00	39.742	3824.0	21.266	39.475	3277.4	18.208
185.00	40.463	4023.5	21.749	40.546	3477.5	18.797
190.00	40.197	4222.6	22.224	41.606	3682.9	19.384
195.00	40.911	4421.4	22.694	42.661	3893.6	19.967
200.00	41.618	4631.8	23.159	43.706	4109.5	20.547
205.00	42.367	4841.8	23.616	44.763	4330.6	21.125
210.00	43.103	5055.4	24.074	45.777	4556.3	21.700
215.00	43.842	5272.8	24.525	46.796	4788.3	22.271
220.00	44.585	5493.9	24.972	47.812	5024.9	22.840
225.00	45.331	5718.7	25.416	48.823	5266.5	23.406
230.00	46.085	5947.2	25.857	49.827	5513.1	23.970
235.00	46.832	6179.5	26.296	50.827	5764.7	24.531
240.00	47.635	6412.7	26.732	51.821	6021.3	25.089
245.00	48.429	6652.9	27.167	52.812	6282.9	25.645
250.00	49.226	6900.0	27.600	53.798	6549.4	26.198
255.00	50.019	7148.2	28.032	54.781	6820.9	26.749
260.00	50.804	7400.2	28.462	55.759	7097.2	27.297
265.00	51.586	7656.2	28.891	56.735	7378.5	27.843
270.00	52.371	7916.1	29.319	57.706	7664.6	28.387
275.00	52.870	8081.6	29.588	58.317	7847.3	28.729
275.00	53.166	8179.4	29.745	58.674	7955.5	28.929
280.00	53.561	8447.8	30.171	59.640	8251.3	29.469
285.00	54.222	8714.8	30.596	60.602	8551.9	30.007
290.00	55.543	8996.1	31.021	61.563	8857.3	30.543
295.00	56.586	9276.7	31.447	62.523	9167.6	31.076
300.00	57.155	9455.9	31.715	63.127	9365.5	31.412
305.00	57.488	9561.9	31.873	63.482	9482.6	31.609

$H_0^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Cole, A. G., Hutchens, J. O., and Stout, J. W.,  
 Heat capacities from 11 to 305°K, and entropies of L-arginine.HCl,  
 L-histidine.HCl, and L-lysine.HCl,  
 J. Phys. Chem. 67, 2245-2247 (1963).

TABLE 14

MOLAL THERMODYNAMIC FUNCTIONS FOR L-ARGININE HYDROCHLORIDE  
 $(\text{NH}_2\text{C}(\text{=NH}_2\text{Cl})\text{NH}(\text{CH}_2)_3\text{(NH}_2\text{)}\text{CHCOOH})$   
 SOLID PHASE

GRAM MOLECULAR WT. = 210.66505 GRAMS

T DEG K = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

T	$c_p^c$	$(H_{T=0}^0 - H_0^0)$	$(H_{T=0}^0 - H_0^0)/T$	$s_T^0$	$-(G_{T=0}^0 - H_0^0)$	$-(G_{T=0}^0 - H_0^0)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.167	0.084	0.017	0.022	0.028	0.006
10.00	0.333	1.321	0.132	0.176	0.444	0.044
15.00	0.500	0.265	0.048	0.163	0.187	0.146
20.00	0.667	17.345	0.867	1.191	6.484	0.324
25.00	0.833	36.660	1.442	2.023	14.034	0.577
30.00	1.000	62.587	2.120	2.018	26.966	0.899
35.00	1.167	100.000	2.843	4.154	44.946	1.231
40.00	1.333	147.515	3.576	5.823	68.877	1.717
45.00	1.500	195.030	4.310	6.705	98.902	2.134
50.00	1.667	242.545	4.840	8.077	135.934	2.717
55.00	1.833	290.060	5.215	9.482	172.73	3.268
60.00	2.000	337.575	5.564	10.303	230.70	3.845
65.00	2.167	385.090	5.869	12.349	286.65	4.444
70.00	2.333	432.605	6.172	13.792	354.20	5.060
75.00	2.500	480.120	6.489	15.229	426.76	5.690
80.00	2.667	527.635	6.717	16.656	506.48	6.331
85.00	2.833	575.150	6.947	18.074	593.32	6.980
90.00	3.000	622.665	7.184	19.420	687.25	7.636
95.00	3.167	670.180	7.424	20.836	785.20	8.297
100.00	3.333	717.695	7.664	22.264	896.08	8.961
105.00	3.500	765.210	7.909	23.626	1010.8	9.627
110.00	3.667	812.725	8.159	24.973	1132.3	10.294
115.00	3.833	860.240	8.414	26.305	1260.5	10.961
120.00	4.000	907.755	8.670	27.621	1395.3	11.628
125.00	4.167	955.270	8.929	28.923	1536.7	12.294
130.00	4.333	1002.785	9.185	30.210	1684.5	12.958
135.00	4.500	1050.300	9.442	31.488	1838.8	13.621
140.00	4.667	1097.815	9.699	32.747	1990.4	14.281
145.00	4.833	1145.330	9.956	34.928	2166.2	14.940
150.00	5.000	1192.845	10.210	35.236	2334.3	15.596
155.00	5.167	1240.360	10.464	36.484	2518.9	16.249
160.00	5.333	1287.875	10.713	37.777	2703.9	16.900
165.00	5.500	1335.390	10.962	38.983	2845.2	17.547
170.00	5.667	1382.905	11.209	40.074	3092.7	18.193
175.00	5.833	1430.420	11.454	41.265	3296.1	18.835
180.00	6.000	1477.935	11.699	42.442	3505.4	19.474
185.00	6.167	1525.450	11.944	43.611	3720.5	20.111
190.00	6.333	1572.965	12.187	44.771	3941.5	20.745
195.00	6.500	1620.480	12.430	45.923	4168.2	21.375
200.00	6.667	1667.995	12.672	47.067	4400.7	22.003
205.00	6.833	1715.510	12.913	48.204	4638.9	22.629
210.00	7.000	1763.025	13.154	49.334	4882.7	23.251
215.00	7.167	1810.540	13.393	50.457	5132.2	23.871
220.00	7.333	1858.055	13.634	51.574	5387.3	24.488
225.00	7.500	1905.570	13.872	52.685	5647.9	25.102
230.00	7.667	1953.085	14.111	53.791	5914.1	25.714
235.00	7.833	2000.600	14.349	54.890	6165.8	26.323
240.00	8.000	2048.115	14.588	55.989	6463.0	26.929
245.00	8.167	2095.630	14.824	57.074	6748.7	27.533
250.00	8.333	2143.145	15.059	58.154	7032.8	28.135
255.00	8.500	2190.660	15.294	59.235	7327.2	28.734
260.00	8.667	2238.175	15.528	60.315	7626.1	29.331
265.00	8.833	2285.690	15.763	61.388	7930.4	29.926
270.00	9.000	2333.205	16.000	62.456	8240.0	30.519
275.00	9.167	2380.720	16.238	63.521	8437.8	30.891
280.00	9.333	2428.235	16.474	64.582	8555.0	31.109
285.00	9.500	2475.750	16.708	65.640	8875.2	31.697
290.00	9.667	2523.265	16.937	66.701	9200.8	32.283
295.00	9.833	2570.780	17.166	67.761	9531.6	32.868
300.00	10.000	2618.295	17.394	68.744	9861.7	33.450
305.00	10.167	2665.810	17.624	69.724	10082.	33.816
310.00	10.333	2713.325	17.853	70.694	10204.	34.030

 $H_{T=0}^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Cole, A. G., Hutchens, J. O. and Stout, J. W.,  
 Heat capacities from 11 to 305 K, and entropies of L-arginine.HCl,  
 L-histidine.HCl, and L-lysine.HCl,  
 J. Phys. Chem. 67, 2245-2247 (1963).

TABLE 15

MOLAL THERMODYNAMIC FUNCTIONS FOR L-HISTIDINE HYDROCHLORIDE  
 $(C_3H_3N_2(HCl)CH_2(NH_2)CHCOOH)$   
 SOLID PHASE

GRAM MOLECULAR WT. = 191.61850 GRAMS  
 $T \text{ DEG K} = 273.15 + T \text{ DEG C}$

1 CAL = 4.1840 JOULES

T DEG K	$C_p^C$ CAL/DEG	$(H_T^0 - H_0^C)$ CAL	$(H_T^0 - H_0^C)/T$ CAL/DEG	$S_T^0$ CAL/DEG	$-(G_T^0 - H_0^C)$ CAL	$-(G_T^0 - H_0^C)/T$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.052	0.066	0.013	0.017	0.022	0.004
10.00	0.117	0.106	0.015	0.039	0.349	0.035
15.00	0.182	0.214	0.038	0.046	0.757	0.117
20.00	0.247	0.284	0.079	0.051	1.438	0.272
25.00	0.312	0.340	0.116	0.072	2.460	0.506
30.00	0.376	0.410	0.156	0.093	3.468	0.816
35.00	0.441	0.480	0.190	0.102	4.459	1.191
40.00	0.504	0.547	0.222	0.117	5.452	1.624
45.00	0.568	0.616	0.250	0.130	6.466	2.104
50.00	0.631	0.675	0.279	0.143	7.482	2.623
55.00	0.694	0.734	0.308	0.151	8.481	3.173
60.00	0.756	0.794	0.336	0.166	9.480	3.749
65.00	0.819	0.853	0.364	0.180	10.479	4.346
70.00	0.882	0.912	0.392	0.194	11.478	4.959
75.00	0.944	0.971	0.419	0.208	12.477	5.584
80.00	1.007	1.030	0.446	0.221	13.476	6.218
85.00	1.069	1.089	0.473	0.231	14.475	6.860
90.00	1.132	1.128	0.500	0.241	15.474	7.507
95.00	1.194	1.177	0.527	0.251	16.473	8.156
100.00	1.256	1.207	0.554	0.261	17.472	8.811
105.00	1.318	1.242	0.581	0.270	18.471	9.465
110.00	1.380	1.282	0.608	0.279	19.470	10.119
115.00	1.442	1.317	0.634	0.288	20.469	10.773
120.00	1.504	1.351	0.661	0.297	21.468	11.425
125.00	1.566	1.381	0.687	0.306	22.467	12.075
130.00	1.628	1.411	0.714	0.315	23.466	12.723
135.00	1.690	1.436	0.737	0.324	24.465	13.369
140.00	1.752	1.461	0.764	0.333	25.464	14.012
145.00	1.814	1.487	0.791	0.342	26.463	14.653
150.00	1.876	1.512	0.818	0.351	27.462	15.290
155.00	1.938	1.537	0.844	0.360	28.461	15.924
160.00	1.999	1.562	0.870	0.369	29.460	16.555
165.00	2.061	1.588	0.897	0.378	30.459	17.183
170.00	2.123	1.612	0.924	0.387	31.458	17.807
175.00	2.184	1.637	0.950	0.396	32.457	18.429
180.00	2.246	1.662	0.977	0.405	33.456	19.047
185.00	2.308	1.687	1.003	0.414	34.455	19.662
190.00	2.370	1.712	1.029	0.423	35.454	20.274
195.00	2.432	1.737	1.055	0.432	36.453	20.882
200.00	2.493	1.762	1.081	0.441	37.452	21.488
205.00	2.555	1.787	1.107	0.450	38.451	22.091
210.00	2.617	1.812	1.132	0.459	39.450	22.690
215.00	2.678	1.837	1.158	0.468	40.449	23.287
220.00	2.740	1.862	1.184	0.477	41.448	23.881
225.00	2.802	1.887	1.209	0.486	42.447	24.472
230.00	2.863	1.912	1.235	0.495	43.446	25.060
235.00	2.925	1.937	1.261	0.504	44.445	25.646
240.00	2.986	1.962	1.287	0.513	45.444	26.229
245.00	3.047	1.987	1.312	0.522	46.443	26.809
250.00	3.109	2.012	1.337	0.531	47.442	27.387
255.00	3.171	2.037	1.363	0.540	48.441	27.962
260.00	3.232	2.062	1.389	0.549	49.440	28.536
265.00	3.293	2.087	1.415	0.558	50.439	29.106
270.00	3.355	2.112	1.440	0.567	51.438	29.675
275.00	3.416	2.137	1.465	0.576	52.437	30.032
280.00	3.478	2.162	1.489	0.585	53.436	30.241
285.00	3.539	2.187	1.515	0.594	54.435	30.805
290.00	3.599	2.212	1.540	0.603	55.434	31.368
295.00	3.661	2.237	1.565	0.612	56.433	31.928
300.00	3.723	2.262	1.589	0.621	57.432	32.486
305.00	3.784	2.287	1.614	0.630	58.431	32.837
310.00	3.845	2.312	1.639	0.639	59.430	33.042

$H_0^C$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Cole, A. G., Hutchens, J. O. and Stout, J. W.,  
 Heat capacities from 11 to 305 K. and entropies of L-arginine.HCl,  
 L-histidine.HCl, and L-lysine.HCl,  
 J. Phys. Chem. 67, 2245-2247 (1963).

TABLE 16

MOIAL THERMODYNAMIC FUNCTIONS FOR L-CYSTINE  
 $(HOOC(NH_2)CH_2CH_2S^-)_2$   
 SOLID PHASE

GRAM MOLECULAR WT. = 240.30154 GRAMS  
 $T \text{ DEG K} = 273.15 + T \text{ DEG C}$

1 CAL = 4.1840 JOULES

T DEG K	C <sub>P</sub> CAL/DEG	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG	S <sub>T</sub> <sup>0</sup> CAL/DEG	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> ) CAL	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>C</sup> )/T CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.050	0.043	0.013	0.017	0.021	0.004
10.00	0.092	0.082	0.022	0.132	0.222	0.033
15.00	0.124	0.108	0.036	0.437	1.602	0.111
20.00	0.160	0.145	0.075	0.981	5.104	0.256
25.00	0.191	0.183	0.123	1.747	11.840	0.474
30.00	0.215	0.218	0.192	2.670	22.867	0.762
35.00	0.232	0.232	0.203	3.766	38.598	1.113
40.00	0.241	0.241	0.213	4.941	60.631	1.517
45.00	0.244	0.247	0.217	6.183	88.477	1.966
50.00	0.241	0.241	0.203	7.475	124.60	2.452
55.00	0.237	0.230	0.181	8.759	163.28	2.965
60.00	0.232	0.228	0.164	10.144	210.63	3.511
65.00	0.227	0.222	0.144	11.503	264.74	4.073
70.00	0.219	0.214	0.217	12.869	325.67	4.652
75.00	0.209	0.204	0.188	14.224	392.43	5.246
80.00	0.201	0.193	0.176	15.596	468.01	5.850
85.00	0.196	0.188	0.149	16.956	549.39	6.463
90.00	0.190	0.184	0.116	18.311	637.56	7.084
95.00	0.182	0.176	0.095	19.655	732.48	7.710
100.00	0.175	0.164	0.064	20.987	834.09	8.341
105.00	0.168	0.152	0.033	22.307	942.34	8.975
110.00	0.161	0.140	0.006	23.616	1057.2	9.610
115.00	0.155	0.127	0.467	24.913	1176.5	10.248
120.00	0.149	0.122	0.316	26.202	1306.3	10.886
125.00	0.144	0.114	0.248	27.478	1440.0	11.524
130.00	0.138	0.104	0.182	28.744	1581.0	12.162
135.00	0.132	0.094	0.121	30.000	1727.0	12.799
140.00	0.126	0.082	0.061	31.247	1881.0	13.436
145.00	0.121	0.074	0.043	32.484	2040.4	14.071
150.00	0.116	0.064	0.006	33.712	2205.9	14.706
155.00	0.111	0.053	0.032	34.931	2377.0	15.330
160.00	0.106	0.041	0.172	36.142	2555.2	15.970
165.00	0.101	0.030	0.045	37.344	2730.9	16.597
170.00	0.096	0.027	0.021	38.535	2920.5	17.227
175.00	0.091	0.024	0.017	39.726	3124.2	17.853
180.00	0.086	0.020	0.013	40.906	3320.8	18.477
185.00	0.082	0.017	0.009	42.075	3533.3	19.093
190.00	0.077	0.014	0.006	43.245	3746.6	19.719
195.00	0.072	0.011	0.004	44.404	3965.7	20.337
200.00	0.068	0.009	0.002	45.557	4190.6	20.953
205.00	0.064	0.006	0.001	46.702	4421.3	21.567
210.00	0.060	0.004	0.000	47.841	4657.7	22.174
215.00	0.057	0.002	0.000	48.973	4899.7	22.789
220.00	0.054	0.001	0.000	50.100	5147.4	23.397
225.00	0.051	0.000	0.000	51.221	5400.7	24.005
230.00	0.049	0.000	0.000	52.336	5659.6	24.607
235.00	0.047	0.000	0.000	53.449	5924.0	25.209
240.00	0.045	0.000	0.000	54.549	6194.0	25.808
245.00	0.043	0.000	0.000	55.649	6469.5	26.406
250.00	0.041	0.000	0.000	56.743	6750.5	27.022
255.00	0.039	0.000	0.000	57.833	7036.9	27.596
260.00	0.037	0.000	0.000	58.919	7328.8	28.188
265.00	0.035	0.000	0.000	60.000	7626.1	28.778
270.00	0.033	0.000	0.000	61.076	7928.8	29.366
275.00	0.030	0.000	0.000	61.752	8122.3	29.736
280.00	0.028	0.000	0.000	62.148	8236.9	29.952
285.00	0.026	0.000	0.000	62.477	8869.0	31.119
290.00	0.024	0.000	0.000	65.336	9193.0	31.700
295.00	0.020	0.000	0.000	66.391	9522.4	32.279
300.00	0.018	0.000	0.000	67.441	9856.9	32.856

<sup>C</sup><sub>T</sub><sup>0</sup> IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Huffman, H. M. and Ellis, E. L.,  
 Thermal data. III. The heat capacities, entropies and free energies of  
 four organic compounds containing sulfur,  
*J. Am. Chem. Soc.* 57, 46-48 (1935).

Hutchens, J. O., Cole, A. G. and Stout, J. W.,  
 Heat capacities and entropies of L-cystine and L-methionine,  
*J. Biol. Chem.* 239, 591-595 (1964).

TABLE 17

MOLAL THERMODYNAMIC FUNCTIONS FOR L-PROLINE  
 $(C_4H_8NCOOH)$   
 SOLID PHASE

GRAM MOLECULAR WT. = 115.13298 GRAMS  
 T DEG K = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

T	$C_p^0$	$(H_T^0 - H_0^0)$	$(H_T^0 - H_0^0)/T$	$S_T^0$	$-(G_T^0 - H_0^0)$	$-(G_T^0 - H_0^0)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.039	0.049	0.010	0.013	0.016	0.003
10.00	0.310	0.780	0.078	0.104	0.261	0.026
15.00	0.981	3.828	0.255	0.342	1.305	0.087
20.00	1.989	11.161	0.558	0.757	3.982	0.194
25.00	3.114	23.900	0.956	1.321	9.126	0.365
30.00	4.267	42.349	1.412	1.991	17.368	0.579
35.00	5.411	66.560	1.902	2.735	29.155	0.833
40.00	6.494	96.553	2.409	3.529	44.798	1.120
45.00	7.512	131.139	2.920	4.353	64.493	1.433
50.00	8.459	171.336	3.427	5.194	88.356	1.767
55.00	9.320	215.83	3.924	6.041	116.44	2.117
60.00	10.144	264.51	4.408	6.888	148.77	2.479
65.00	10.912	317.17	4.880	7.731	185.32	2.851
70.00	11.667	373.51	5.336	8.565	226.06	3.229
75.00	12.372	433.21	5.776	9.389	270.95	3.613
80.00	12.934	496.24	6.203	10.202	314.93	3.999
85.00	13.453	562.48	6.617	11.005	372.46	4.388
90.00	14.129	631.69	7.019	11.746	424.96	4.777
95.00	14.675	702.72	7.408	12.575	490.90	5.167
100.00	15.194	778.40	7.784	13.341	555.69	5.557
105.00	15.703	852.64	8.149	14.095	624.29	5.946
110.00	16.215	933.43	8.504	14.837	696.62	6.333
115.00	16.731	1017.8	8.850	15.569	774.64	6.719
120.00	17.244	1102.7	9.189	16.292	852.29	7.102
125.00	17.748	1190.2	9.522	17.006	935.54	7.464
130.00	18.256	1280.4	9.848	17.712	1022.3	7.864
135.00	18.767	1372.6	10.169	18.411	1112.6	8.242
140.00	19.275	1467.9	10.485	19.102	1206.4	8.617
145.00	19.787	1565.5	10.797	19.788	1303.7	8.991
150.00	20.314	1665.8	11.105	20.467	1404.3	9.362
155.00	20.848	1768.7	11.411	21.142	1508.3	9.731
160.00	21.379	1874.3	11.714	21.812	1615.7	10.098
165.00	21.917	1982.5	12.015	22.478	1726.4	10.463
170.00	22.458	2093.3	12.314	23.140	1840.5	10.826
175.00	22.976	2206.9	12.611	23.758	1957.8	11.188
180.00	23.518	2325.1	12.906	24.453	2078.5	11.547
185.00	24.051	2442.0	13.200	25.105	2202.4	11.905
190.00	24.597	2560.7	13.493	25.754	2329.5	12.261
195.00	25.142	2688.0	13.785	26.409	2459.9	12.615
200.00	25.541	2814.9	14.075	27.042	2593.5	12.968
205.00	26.156	2944.4	14.363	27.682	2730.3	13.319
210.00	26.678	3076.5	14.650	28.315	2870.3	13.668
215.00	27.210	3211.2	14.936	28.942	3013.5	14.016
220.00	27.744	3346.6	15.221	29.584	3159.8	14.363
225.00	28.274	3486.6	15.505	30.213	3309.3	14.708
230.00	28.793	3631.3	15.788	30.840	3462.0	15.052
235.00	29.306	3776.6	16.070	31.465	3617.7	15.395
240.00	29.824	3924.4	16.352	32.087	3776.6	15.736
245.00	30.330	4074.3	16.632	32.708	3938.6	16.076
250.00	30.847	4221.9	16.912	33.326	4103.7	16.415
255.00	31.429	4368.7	17.191	33.943	4271.9	16.752
260.00	31.964	4514.2	17.470	34.569	4443.1	17.089
265.00	32.505	4670.4	17.749	35.173	4617.4	17.424
270.00	33.137	4867.2	18.027	35.785	4794.8	17.759
275.00	33.371	4971.8	18.202	36.171	4908.2	17.969
280.00	33.568	5083.7	18.304	36.396	4975.3	18.092
285.00	34.102	5202.9	18.592	37.006	5158.8	18.424
290.00	34.642	5374.8	18.859	37.514	5345.3	18.756
295.00	35.150	5547.3	19.136	38.222	5534.9	19.086
300.00	35.748	5726.7	19.412	38.826	5727.6	19.415
305.00	36.106	5899.8	19.587	39.210	5850.5	19.623
310.00	36.319	5906.8	19.689	39.434	5923.2	19.744

$H_0^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG K AND 1 ATM PRESSURE.

Huffman, H. M. and Fox, S. W.,  
 Thermal data. XIII. The heat capacities and entropies of creatine hydrate,  
 dl-citrulline, dl-ornithine, l-proline and taurine,  
*J. Am. Chem. Soc.* 62, 3464-3465 (1940).

Cole, A. G., Hutchens, J. O. and Stout, J. W.,  
 Heat capacities from 11 to 305 K. and entropies of l-phenylalanine,  
 l-proline, l-tryptophane, and l-tryrosine. Some free energies of formation,  
*J. Phys. Chem.* 67, 1892-1855 (1963).

## Section II

### Heats and Free Energies of Formation of Compounds of C, H, N, O, P, and S

E. S. Domalski and George T. Armstrong

The data on the accompanying tables were obtained by a search of the references listed, each of which is a competent review of thermodynamic data covering many of the compounds of interest. Where data were available in Reference 1 they were used. Values found in Reference 2 were taken if information was not found in the other references. The list is given in the Appendix of NBS Report 8521 and was used as a basis for the search. Only a few compounds were included in the table which were not on the original list. On this account, the list of compounds is by no means complete, and it will be augmented in the future. While data in Table 1 may be expected to be the best available for most of the compounds, new data may be available for a few, and not have been included in the reviews searched. Estimates of the uncertainties which should be ascribed to the data have not yet been made here. Absence of data for a compound listed in the table does not necessarily, at this stage of the study, mean that no measurements have been made on the compound. We have had no way of indicating partial data, insufficient for calculation of enthalpy or free energy of formation. In addition, as mentioned before, very recent publications have not been covered thus far in the search.

TABLE I

Preliminary Table of Selected Thermodynamic Data on Compounds of CHNOPS  
 Containing Not More Than One C Atom per Molecule

Empirical Formula	Functional Group Formula	Name	State	$\Delta H^\circ_{298}$	$\Delta F^\circ_{298}$	$S^\circ_{298}$	Ref.
				kcal mole <sup>-1</sup>	kcal mole <sup>-1</sup>	cal mole <sup>-1</sup> deg <sup>-1</sup>	
C	C	carbon, monatomic graphite diamond	g c c	171.291 0 0.4533	160.442 0 0.6930	37.760 1.372 0.568	[1] [1] [1]
CH	CH	methylidyne	g	142.1			[4]
CHN	HCN	hydrogen cyanide	g l	31.2 25.2	28.7 29.0	48.23 26.97	[2] [2]
		hydrocyanic acid,	m=l	aq	25.2	26.8	30.8
CHNO	HCNO	hydrogen cyanate	g				
CHNO	HCNO	cyanic acid,	m=l	aq	-35.1	-28.9	43.6
CHNS	HCNS	hydrogen thiocyanate thiocyanic acid,	m=l	g aq	17.7		
CH <sub>3</sub> O <sub>6</sub>	CH(NO <sub>2</sub> ) <sub>3</sub>	trinitromethane	l		-18.6		[2]
CHO	CHO	formyl	g	-2.900	-6.543	53.683	[4]
CH <sub>2</sub>	CH <sub>2</sub>	methylene	g	95.000	91.809	43.271	[11]
CH <sub>2</sub> N <sub>2</sub>	(NH <sub>2</sub> )CN	cyanamide	800 H <sub>2</sub> O	c aq	9.2 12.9		[2] [2]
CH <sub>2</sub> N <sub>2</sub>	(CH <sub>2</sub> )N <sub>2</sub>	diazomethane	g				
CH <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	(NO <sub>2</sub> )CH(:NOH)	formonitriolic acid	c				
CH <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	CH <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	dinitromethane	l				
CH <sub>2</sub> N <sub>4</sub>	NHN:NCH:N	1,2,3,5-tetrazole	c				
CH <sub>2</sub> O	HCHO	formaldehyde	60 H <sub>2</sub> O 40 CH <sub>3</sub> OH	g aq	-27.700 -42.5 -42.7	-26.266	52.261
(CH <sub>2</sub> O)x	(CH <sub>2</sub> O)x	paraformaldehyde	c				
CH <sub>2</sub> O <sub>2</sub>	HCOOH	formic acid	g l m=l 0.2 H <sub>2</sub> O 0.5 H <sub>2</sub> O 1.0 H <sub>2</sub> O 1.5 H <sub>2</sub> O 2.0 H <sub>2</sub> O 2.5 H <sub>2</sub> O 4 H <sub>2</sub> O 5 H <sub>2</sub> O 10 H <sub>2</sub> O 15 H <sub>2</sub> O 25 H <sub>2</sub> O 50 H <sub>2</sub> O 100 H <sub>2</sub> O 200 H <sub>2</sub> O $\infty$ H <sub>2</sub> O	aq aq aq aq aq aq aq aq aq aq aq aq aq aq aq aq aq	-86.67 -97.8 -98.0 -97.86 -97.93 -98.00 -98.01 -97.99 -97.99 -97.98 -97.96 -97.94 -97.93 -97.94 -97.95 -97.96 -97.97 -98.0	-80.24 -82.7 -85.1 -97.8 -97.93 -98.00 -98.01 -97.99 -97.99 -97.98 -97.96 -97.94 -97.93 -97.94 -97.95 -97.96 -97.97 -98.0	60.0 30.82 39.1
CH <sub>2</sub> O <sub>3</sub>	H <sub>2</sub> CO <sub>3</sub>	carbonic acid undissociated,	m=l	aq	-167.17	-148.94	45.0
CH <sub>2</sub> S <sub>3</sub>	H <sub>2</sub> CS <sub>3</sub>	trithiocarbonic acid	aq				
CH <sub>3</sub>	CH <sub>3</sub>	methyl	g	31.940	32.546	46.137	[8]
CH <sub>3</sub> NO	HCONH <sub>2</sub>	formamide	l aq	-61.6 -56.0			[2] [2]
CH <sub>3</sub> NO	H <sub>2</sub> S(:NOH)	formaldehyde oxime	l				
CH <sub>3</sub> NO <sub>2</sub>	CH <sub>3</sub> NO <sub>2</sub>	nitromethane	l aq	-21.28 -20.7	2.26	41.1	[2] [2]

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_{f298}^\circ$ kcal mole <sup>-1</sup>	$\Delta F_{f298}^\circ$ kcal mole <sup>-1</sup>	$S_{298}^\circ$ cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.	
CH <sub>5</sub> NO	CH <sub>3</sub> ONH <sub>2</sub>	methoxyamine	c aq					
CH <sub>5</sub> NO <sub>2</sub>	HCOONH <sub>4</sub>	ammonium formate	c aq	-132.8 -129.83			[2] [2]	
CH <sub>5</sub> NO <sub>3</sub>	NH <sub>4</sub> HCO <sub>3</sub>	ammonium bicarbonate	m=1	c aq	-203.7 -196.92	-159.31	49.7	[2] [2]
CH <sub>5</sub> N <sub>3</sub>	NH <sub>2</sub> C(NH)NH <sub>2</sub>	guanidine		c aq	-17.0 -18.3		[2] [2]	
CH <sub>5</sub> N <sub>3</sub> O	NH <sub>2</sub> CONHNH <sub>2</sub>	semicarbazide	c aq					
CH <sub>5</sub> N <sub>3</sub> O <sub>3</sub> S	NH <sub>2</sub> CSNH <sub>2</sub> •HNO <sub>3</sub>	thiourea nitrate	c	-74.5			[2]	
CH <sub>5</sub> N <sub>3</sub> O <sub>4</sub>	NH <sub>2</sub> CONH <sub>2</sub> •HNO <sub>3</sub>	urea nitrate	c aq	-114.8			[2]	
CH <sub>5</sub> N <sub>3</sub> S	NH <sub>2</sub> CSNHNH <sub>2</sub>	thiosemicarbazide	c aq					
CH <sub>5</sub> O <sub>3</sub> P	CH <sub>3</sub> PO(OH) <sub>2</sub>	methyl phosphonic acid	c aq					
CH <sub>5</sub> P	CH <sub>3</sub> PH <sub>2</sub>	methyl phosphine	g l					
CH <sub>6</sub> N <sub>2</sub>	CH <sub>3</sub> NHHN <sub>2</sub>	methyl hydrazine	g l					
CH <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	NH <sub>2</sub> COONH <sub>4</sub>	ammonium carbamate	c aq	-154.21 -150.4	-109.47	39.70	[2] [2]	
CH <sub>6</sub> N <sub>4</sub>	NH <sub>2</sub> C(NH)NNH <sub>2</sub>	1-aminoguanidine	c aq					
CH <sub>6</sub> N <sub>4</sub> O	CO(NHNH <sub>2</sub> ) <sub>2</sub>	carbohydrazide	c					
CH <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	(NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub>	ammonium carbonate	c aq	-225.11	-164.22	41.2	[2]	
CH <sub>12</sub> O <sub>8</sub>	CO <sub>2</sub> •6H <sub>2</sub> O	carbon dioxide hexahydrate	c	-520			[2]	
CH <sub>16</sub> O <sub>6</sub>	CH <sub>4</sub> •6H <sub>2</sub> O	methane hexahydrate	c	-445			[2]	
CN	CN	cyanogen	g	109.000	101.796	48.406	[8]	
(CN) <sub>x</sub>	(CN) <sub>x</sub>	paracyanogen	c					
CN <sub>4</sub>	CN(N <sub>3</sub> )	cyanogen azide	c	92.6			[2]	
$\frac{1}{x}$ (CN <sub>4</sub> ) <sub>x</sub>	$\frac{1}{x}$ (CN(N <sub>3</sub> )) <sub>x</sub>	paracyanogen azide	c	82.2			[2]	
CN <sub>4</sub> O <sub>8</sub>	C(NO <sub>2</sub> ) <sub>4</sub>	tetraniromethane	l	8.8			[2]	
CO	CO	carbon monoxide	g	-26.416	-32.780	42.214	[1]	
COS	COS	carbonyl sulfide	g	-33.080	-39.589	55.323	[4]	
CO <sub>2</sub>	CO <sub>2</sub>	carbon dioxide	g	-94.051	-94.261	51.072	[1]	
		undissociated, m=1	aq	-98.85	-92.26	28.3	[1]	
CP	CP	carbon phosphide	g	111.700	98.327	51.661	[6]	
CS	CS	carbon monosulfide	g	55.000	42.684	50.299	[8]	
CS <sub>2</sub>	CS <sub>2</sub>	carbon disulfide	l	27.980	15.991	56.832	[5]	
C <sub>2</sub>	C <sub>2</sub>	carbon diatomic	g	199.026	185.636	47.628	[6]	
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	N <sub>2</sub> H <sub>4</sub> •(HCOOH) <sub>2</sub>	hydrazine formate	c aq					
C <sub>2</sub> N <sub>2</sub>	(CN) <sub>2</sub>	cyanogen	g	73.870	71.117	57.711	[4]	

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_f^{\circ}$	$\Delta F_f^{\circ}$	$S_f^{\circ}$	Ref.
				kcal mole <sup>-1</sup>	kcal mole <sup>-1</sup>	cal mole <sup>-1</sup> deg <sup>-1</sup>	
C <sub>3</sub>	C <sub>3</sub>	carbon, triatomic	g	189.670	175.777	50.688	[3]
C <sub>3</sub> O <sub>2</sub>	C <sub>3</sub> O <sub>2</sub>	carbon suboxide	g	-8.300	-10.726	61.236	[3]
C <sub>3</sub> S <sub>2</sub>	C <sub>3</sub> S <sub>2</sub>	carbon subsulfide	g				
C <sub>4</sub>	C <sub>4</sub>	carbon, tetratomic	g	242.321	226.629	58.083	[3]
C <sub>4</sub> N <sub>2</sub>	C <sub>2</sub> (CN) <sub>2</sub>	carbon subnitride	g	122.900	113.575	67.936	[3]
C <sub>5</sub>	C <sub>5</sub>	carbon, pentatomic	g	242.374	226.634	59.608	[3]
H	H	hydrogen monatomic	g	52.095	48.580	27.391	[1]
HN	HN	imidogen	g	79.200	77.765	43.297	[3]
HN <sub>3</sub>	HN <sub>3</sub>	hydrogen azide	g	70.3	78.4	57.09	[1]
		hydrazoic acid undissociated, m=1	aq	63.1	78.2	33.6	[1]
				62.16	76.9	34.9	[1]
HNO	HNO	nitroxyl	g	23.800	26.859	52.729	[9]
HNO <sub>2</sub>	HNO <sub>2</sub>	cis hydrogen nitrite trans hydrogen nitrite hydrogen nitrite (cis-trans mixture)	g	-18.64	-10.27	59.43	[1]
		nitrous acid	g	-19.15	-10.82	59.54	[1]
			aq				
			g	-19.0	-11.0	60.7	[1]
			g	-28.5	-13.3	36.5	[1]
HNO <sub>3</sub>	HNO <sub>3</sub>	hydrogen nitrate	g	-32.28	-17.87	63.64	[1]
		nitric acid, m=1	g	-41.61	-19.31	37.19	[1]
			aq	-49.56	-26.61	35.0	[1]
			1 H <sub>2</sub> O	-44.845			
			2 H <sub>2</sub> O	-46.500			
			3 H <sub>2</sub> O	-47.459			
			5 H <sub>2</sub> O	-48.462			
			10 H <sub>2</sub> O	-49.192			
			25 H <sub>2</sub> O	-49.430			
			50 H <sub>2</sub> O	-49.439			
			100 H <sub>2</sub> O	-49.440			
			500 H <sub>2</sub> O	-49.468			
			1000 H <sub>2</sub> O	-49.484			
			5000 H <sub>2</sub> O	-49.518			
			10000 H <sub>2</sub> O	-49.529			
			50000 H <sub>2</sub> O	-49.545			
H <sub>3</sub> NO <sub>4</sub>	HNO <sub>3</sub> •H <sub>2</sub> O	nitric acid hydrate	l	-112.960	-78.410	51.83	[2]
HNO <sub>5</sub>	(NO)HSO <sub>4</sub>	nitrosyl sulfuric acid	c				
HO	OH	hydroxyl	g	9.31	8.18	43.890	[1]
HO <sub>2</sub>	HO <sub>2</sub>	hydroperoxy	g	5.000	8.049	54.383	[10]
HP	PH	phosphorus monohydride	g	59.170	51.467	46.891	[7]
HP <sub>2</sub>	P <sub>2</sub> H	diphosphorus monohydride	c	-14.5			[2]
HPO <sub>3</sub>	HPO <sub>3</sub>	metaphosphoric acid	c	-226.7			[1]
			aq	-233.5			[1]
HS	SH	sulfur monohydride	g	32.000	24.990	46.745	[3]
H <sub>2</sub>		hydrogen	g	0 -1.0	0 4.2	31.208 13.8	[1]
H <sub>2</sub> N	NH <sub>2</sub>	amidogen	g	40.300	42.976	45.113	[3]
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	hyponitrous acid, m=1	aq	-13.7	8.4	52	[2]
H <sub>2</sub> O	H <sub>2</sub> O	water	g	-57.796 -68.315	-54.635 -56.688	45.104 16.71	[1]
H <sub>2</sub> O <sub>2</sub>	H <sub>2</sub> O <sub>2</sub>	hydrogen peroxide	g	-32.58	-25.25	55.6	[1]
		m=1	g	-44.88	-28.78	26.2	[1]
			aq	-45.69	-32.05	34.4	[1]
			0.5 H <sub>2</sub> O	-45.198			
			1 H <sub>2</sub> O	-45.365			
			5 H <sub>2</sub> O	-45.638			
			10 H <sub>2</sub> O	-45.670			
			50 H <sub>2</sub> O	-45.687			

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_f^{\circ}$ 298 kcal mole <sup>-1</sup>	$\Delta F_f^{\circ}$ 298 kcal mole <sup>-1</sup>	$S_f^{\circ}$ 298 cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.
H <sub>2</sub> P	PH <sub>2</sub>	phosphorus dihydride	g	30.100	25.884	50.800	[12]
H <sub>2</sub> S	H <sub>2</sub> S	hydrogen sulfide hydrosulfuric acid	g aq	-4.93 -9.5	-8.02 -6.66	49.16 29	[1] [1]
H <sub>2</sub> S <sub>2</sub>	H <sub>2</sub> S <sub>2</sub>	hydrogen disulfide	l	-5.5			[2]
H <sub>2</sub> S <sub>3</sub>	H <sub>2</sub> S <sub>3</sub>	hydrogen trisulfide	g				
H <sub>2</sub> S <sub>5</sub>	H <sub>2</sub> S <sub>5</sub>	hydrogen pentasulfide	l	0.7			[2]
H <sub>2</sub> SO <sub>3</sub>	H <sub>2</sub> SO <sub>3</sub>	sulfurous acid undissociated, m=1	aq	-145.51	-128.56	55.5	[1]
		100 H <sub>2</sub> O	aq	-146.369			[1]
		200 H <sub>2</sub> O	aq	-146.670			[1]
		500 H <sub>2</sub> O	aq	-147.126			[1]
		1000 H <sub>2</sub> O	aq	-147.516			[1]
		2000 H <sub>2</sub> O	aq	-147.957			[1]
		5000 H <sub>2</sub> O	aq	-148.524			[1]
		10000 H <sub>2</sub> O	aq	-148.899			[1]
H <sub>2</sub> SO <sub>4</sub>	H <sub>2</sub> SO <sub>4</sub>	sulfuric acid	l m=1	-194.548 -217.32	-164.942 -177.97	37.501 4.8	[1] [1]
		1 H <sub>2</sub> O	aq	-201.193			[1]
		2 H <sub>2</sub> O	aq	-204.425			[1]
		3 H <sub>2</sub> O	aq	-206.241			[1]
		4 H <sub>2</sub> O	aq	-207.428			[1]
		5 H <sub>2</sub> O	aq	-208.288			[1]
		6 H <sub>2</sub> O	aq	-208.944			[1]
		8 H <sub>2</sub> O	aq	-209.865			[1]
		10 H <sub>2</sub> O	aq	-210.451			[1]
		15 H <sub>2</sub> O	aq	-211.191			[1]
		25 H <sub>2</sub> O	aq	-211.660			[1]
		50 H <sub>2</sub> O	aq	-211.941			[1]
		75 H <sub>2</sub> O	aq	-212.068			[1]
		100 H <sub>2</sub> O	aq	-212.150			[1]
		115 H <sub>2</sub> O	aq	-212.192			[1]
		200 H <sub>2</sub> O	aq	-212.387			[1]
		300 H <sub>2</sub> O	ad	-212.565			[1]
		500 H <sub>2</sub> O	ad	-212.833			[1]
		800 H <sub>2</sub> O	ad	-213.128			[1]
		1000 H <sub>2</sub> O	ad	-213.275			[1]
		1500 H <sub>2</sub> O	ad	-213.552			[1]
		2000 H <sub>2</sub> O	ad	-213.740			[1]
		3000 H <sub>2</sub> O	ad	-214.015			[1]
		5000 H <sub>2</sub> O	ad	-214.390			[1]
		10000 H <sub>2</sub> O	ad	-215.060			[1]
		20000 H <sub>2</sub> O	ad	-215.880			[1]
		50000 H <sub>2</sub> O	ad	-216.545			[1]
		100000 H <sub>2</sub> O	ad	-216.875			[1]
		500000 H <sub>2</sub> O	ad	-217.189			[1]
H <sub>2</sub> SO <sub>5</sub>	H <sub>2</sub> SO <sub>5</sub>	peroxymonosulfuric acid	c				
H <sub>2</sub> S <sub>2</sub> O <sub>4</sub>	H <sub>2</sub> S <sub>2</sub> O <sub>4</sub>	dithionous acid	aq	-164			[2]
H <sub>2</sub> S <sub>2</sub> O <sub>6</sub>	H <sub>2</sub> S <sub>2</sub> O <sub>6</sub>	dithionic acid	aq	-280.0			[2]
H <sub>2</sub> S <sub>2</sub> O <sub>7</sub>	H <sub>2</sub> S <sub>2</sub> O <sub>7</sub>	pyrosulfuric acid	c	-304.4			[1]
H <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	H <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	peroxydisulfuric acid, m=1	aq	-320.0	-265.4	59.3	[2]
H <sub>3</sub> N	NH <sub>3</sub>	ammonia undissociated, m=1	g aq	-11.07 -19.19	-3.94 -6.35	45.97 26.6	[1] [1]
		1 H <sub>2</sub> O	aq	-18.011			[1]
		2 H <sub>2</sub> O	aq	-18.560			[1]
		5 H <sub>2</sub> O	aq	-18.945			[1]
		10 H <sub>2</sub> O	aq	-19.074			[1]
		20 H <sub>2</sub> O	aq	-19.125			[1]
		50 H <sub>2</sub> O	aq	-19.156			[1]
		100 H <sub>2</sub> O	aq	-19.167			[1]
		500 H <sub>2</sub> O	aq	-19.173			[1]
		1000 H <sub>2</sub> O	aq	-19.171			[1]
		5000 H <sub>2</sub> O	aq	-19.154			[1]
		10000 H <sub>2</sub> O	aq	-19.140			[1]
		50000 H <sub>2</sub> O	aq	-19.086			[1]

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_f^{\circ}$ kcal mole <sup>-1</sup>	$\Delta F_f^{\circ}$ kcal mole <sup>-1</sup>	$S_f^{\circ}$ cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.	
H <sub>3</sub> NO	NH <sub>2</sub> OH	hydroxylamine	c aq	-27.3 -23.5			[1]	
H <sub>3</sub> NO <sub>3</sub> S	(NH <sub>2</sub> )SO <sub>3</sub> H	sulfamic acid	c aq	-161.3 -156.3			[1]	
H <sub>3</sub> O <sub>2</sub> P	H <sub>3</sub> PO <sub>2</sub>	hypophosphorous acid	c 200 H <sub>2</sub> O	-144.5 -144.4			[1]	
H <sub>3</sub> O <sub>3</sub> P	H <sub>3</sub> PO <sub>3</sub>	orthophosphorous acid	c aq	-228.3 -228.4			[1]	
H <sub>3</sub> O <sub>4</sub> P	H <sub>3</sub> PO <sub>4</sub>	orthophosphoric acid	c l 1 H <sub>2</sub> O 1.5 H <sub>2</sub> O 2 H <sub>2</sub> O 3 H <sub>2</sub> O 4 H <sub>2</sub> O 5 H <sub>2</sub> O 7 H <sub>2</sub> O 10 H <sub>2</sub> O 20 H <sub>2</sub> O 50 H <sub>2</sub> O 100 H <sub>2</sub> O 200 H <sub>2</sub> O 500 H <sub>2</sub> O 1000 H <sub>2</sub> O 2000 H <sub>2</sub> O 3000 H <sub>2</sub> O 5000 H <sub>2</sub> O 10000 H <sub>2</sub> O	-305.7 -302.8 -307.92 -304.69 -305.26 -305.60 -306.23 -306.60 -306.87 -307.20 -307.48 -307.831 -308.067 -308.176 -308.276 -308.403 -308.532 -308.696 -308.818 -308.982 -309.197	-267.5 -273.10	26.41 37.8		[1]
H <sub>3</sub> P	PH <sub>3</sub>	phosphine	g aq	1.3 -2.16	3.2 0.35	50.22 48.2	[1]	
H <sub>4</sub> N <sub>2</sub>	N <sub>2</sub> H <sub>4</sub>	hydrazine	g l undissociated, m=l aq	22.80 12.10 8.20	38.07 35.67 30.6	56.97 28.97 33	[1]	
H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	NH <sub>4</sub> NO <sub>2</sub>	ammonium nitrite	m=l c aq	-61.3 -56.7	-27.9	60.6	[1]	
H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	NH <sub>4</sub> NO <sub>3</sub>	ammonium nitrate	c,V m=l 3 H <sub>2</sub> O 5 H <sub>2</sub> O 10 H <sub>2</sub> O 25 H <sub>2</sub> O 50 H <sub>2</sub> O 100 H <sub>2</sub> O 500 H <sub>2</sub> O 1000 H <sub>2</sub> O 5000 H <sub>2</sub> O 10000 H <sub>2</sub> O	-87.38 -81.23 -83.485 -83.050 -82.470 -81.866 -81.538 -81.318 -81.183 -81.177 -81.194 -81.202	-43.98 -43.58	36.11 62.1	[1]	
H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>	NH <sub>2</sub> OH•HNO <sub>3</sub>	hydroxylamine nitrate	c aq	-87.6 -82.4			[1]	
H <sub>4</sub> N <sub>4</sub>	NH <sub>4</sub> N <sub>3</sub>	ammonium azide	m=l c aq	27.6 34.1	65.5 64.3	26.9 52.7	[1]	
H <sub>4</sub> O <sub>4.5</sub> P	H <sub>3</sub> PO <sub>4</sub> • <sub>1/2</sub> H <sub>2</sub> O	phosphoric acid hemihydrate	c l	-342.1 -339.3	-296.9	30.87	[1]	
H <sub>4</sub> O <sub>5</sub> S	H <sub>2</sub> SO <sub>4</sub> •H <sub>2</sub> O	sulfuric acid hydrate	l	-269.508	-227.186	50.56	[1]	
H <sub>4</sub> P <sub>2</sub>	P <sub>2</sub> H <sub>4</sub>	diphosphine	g l	5.0 -1.2			[1]	
H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	H <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	pyrophosphoric acid supercooled	m=l 500 H <sub>2</sub> O aq	-535.6 -533.4 -542.2 -543.0	-486.8	68	[1]	

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_{f298}^\circ$ kcal mole <sup>-1</sup>	$\Delta F_{f298}^\circ$ kcal mole <sup>-1</sup>	$S_{298}^\circ$ cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.
$H_5NO$	$NH_4OH$	ammonium hydroxide	$l$	-86.33	-60.74	39.57	[1]
		undissociated, m=1	aq	-87.505	-63.04	43.3	[1]
		ionized, m=1	aq	-86.64	-56.56	24.5	[1]
$H_5NS$	$NH_4SH$	ammonium hydrosulfide	c	-37.5	-12.1	23.3	[1]
		200 $H_2O$	aq	-34.8			[1]
$H_5NO_3S$	$NH_4HSO_3$	ammonium bisulfite	c	-183.7			[1]
		300 $H_2O$	aq	-181.3			[1]
$H_5NO_4S$	$NH_4HSO_4$	ammonium bisulfate	c	-245.45			[1]
		200 $H_2O$	aq	-245.65			[1]
$H_5NO_5S$	$NH_2OH \cdot H_2SO_4$	hydroxylamine sulfate	aq	-246.7			[1]
$H_5N_3O_3$	$N_2H_4 \cdot HNO_3$	hydrazine nitrate	m=1	-60.13			[1]
$H_6NO_2P$	$(NH_4)H_2PO_2$	ammonium hypophosphite	c				
		aq					
$H_6NO_3P$	$(NH_4)H_2PO_3$	ammonium orthophosphite	c				
$H_6NO_4P$	$(NH_4)H_2PO_4$	primary ammonium orthophosphate	c	-345.94	-289.89	36.32	[1]
		m=1	aq	-342.05	-289.70	48.7	[1]
		15 $H_2O$	aq	-342.157			[1]
		50 $H_2O$	aq	-342.113			[1]
		100 $H_2O$	aq	-342.088			[1]
		500 $H_2O$	aq	-342.059			[1]
		1000 $H_2O$	aq	-342.055			[1]
		$\infty H_2O$	aq	-342.05			[1]
$H_6N_2O$	$N_2H_4 \cdot H_2O$	hydrazine hydrate	g	-49.0	-18.9	63	[1]
		undissociated, m=1	aq	-58.01	-26.1	49.7	[1]
$H_6N_2O_3S$	$(NH_2)_2SO_3NH_4$	ammonium sulfamate	c				
$H_6N_2O_4S$	$N_2H_4 \cdot H_2SO_4$	hydrazine sulfate	c	-231.6			[2]
		1000 $H_2O$	aq	-223.44			[2]
$H_6P_{12}$	$(P_2H_4)_3$	diphosphine trimer	c				
$H_{6.5}O_{8.5}P_2$	$H_4P_2O_7 \cdot H_2O$	pyrophosphoric acid hydrate	c	-640.9			[1]
$H_7NO_6$	$HNO_3 \cdot 3H_2O$	nitric acid trihydrate	$l$	-252.203	-193.701	82.92	[2]
$H_7N_2O_3P$	$N_2H_4 \cdot H_3PO_3$	hydrazine orthophosphite	c				
$H_7N_2O_4P$	$N_2H_4 \cdot H_3PO_4$	hydrazine orthophosphate	c				
		aq					
$H_8N_2O_3S$	$(NH_4)_2SO_3$	ammonium sulfite	c	-211.6			[1]
$H_8N_2O_3S_2$	$(NH_4)_2S_2O_3$	ammonium thiosulfate	c	-211.0			[1]
		aq					
$H_8N_2O_4S$	$(NH_4)SO_4$	ammonium sulfate	c	-282.23	-215.56	52.6	[1]
		m=1	aq	-280.66	-215.77	58.6	[1]
		10 $H_2O$	aq	-280.72			[1]
		50 $H_2O$	aq	-280.51			[1]
		100 $H_2O$	aq	-280.407			[1]
		500 $H_2O$	aq	-280.242			[1]
$H_8N_2O_5S_2$	$(NH_4)_2S_2O_5$	ammonium pyrosulfite, m=1	aq	-295.3			[2]
$H_8N_2O_6P_2$	$N_2H_4 \cdot H_4P_2O_6$	hydrazine hypophosphite	c				
$H_8N_2O_6S$	$2NH_2OH \cdot H_2SO_4$	dihydroxylamine sulfate	aq	-281.3			[1]
$H_8N_2O_6S_2$	$(NH_4)_2S_2O_6$	ammonium dithionate	c				
		aq					

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_{f298}^\circ$ kcal mole <sup>-1</sup>	$\Delta F_{f298}^\circ$ kcal mole <sup>-1</sup>	$S_{298}^\circ$ cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.
$H_8N_2O_7S_2$	$(NH_4)_2S_2O_7$	ammonium pyrosulfate	c aq				
$H_8N_2O_8S_2$	$(NH_4)_2S_2O_8$	ammonium peroxydisulfate	c aq	-392.5 -383.3			[1] [1]
$H_8N_2S$	$(NH_4)_2S$	ammonium monosulfide	aq	-34.5			[2]
$H_8N_2S_4$	$(NH_4)_2S_4$	ammonium tetrasulfide	c aq	-67.4 -60.0			[2] [2]
$H_8N_2S_5$	$(NH_4)_2S_5$	ammonium pentasulfide	c aq	-68.8 -61.2			[2] [2]
$H_8O_4SP_2$	$(PH_4)_2SO_4$	phosphonium sulfate	c aq				
$H_9N_2O_4P$	$(NH_4)_2HPO_4$	secondary ammonium orthophosphate	c aq 15 H <sub>2</sub> O 50 H <sub>2</sub> O 100 H <sub>2</sub> O 500 H <sub>2</sub> O 1000 H <sub>2</sub> O	-374.50 -372.71 -370.40 -370.85 -371.22 -371.4 -371.44	-298.85	46.2	[1] [1] [1] [1] [1] [1] [1]
$H_{10}N_2O_4S$	$(NH_4)_2SO_3 \cdot H_2O$	ammonium sulfite hydrate	c	-283.8			[1]
$H_{10}N_2O_6P$	$N_2H_4 \cdot 2H_3PO_3$	hydrazine diorthophosphite	c aq				
$H_{10}N_2O_6P_2$	$(NH_4)_2H_2P_2O_6$	diammonium hypophosphate	c aq				
$H_{10}N_4O_4S$	$(N_2H_4)_2H_2SO_4$	dihydrazine sulfate	c m=1 aq	-229.2 -221.0	-138.5	77	[1] [1]
$H_{12}N_3O_4P$	$(NH_4)_3PO_4$	tertiary ammonium orthophosphate	c 600 H <sub>2</sub> O aq	-299.6 -391.3			[1] [1]
$H_{12}N_4O_5S$	$(N_2H_4)_2H_2SO_4 \cdot H_2O$	dihydrazine sulfate hydrate	c	-291.3			[1]
$H_{14}O_6S$	$H_2S \cdot 6H_2O$	hydrogen sulfide hexahydrate	c	-431.2			[2]
$H_{15}O_6P$	$PH_3 \cdot 6H_2O$	phosphine hexahydrate	c	-422.7			[2]
$H_{18}N_3O_7P$	$(NH_4)_3PO_4 \cdot 3H_2O$	tertiary ammonium orthophosphate trihydrate	c	-410.8			[1]
N	N	nitrogen monatomic	g	112.979	108.883	36.622	[1]
NO	NO	nitric oxide	g	21.57	20.69	50.35	[1]
NO <sub>2</sub>	NO <sub>2</sub>	nitrogen dioxide	g	277.4			[1]
NO <sub>3</sub>	NO <sub>3</sub>	nitrogen trioxide	g	13.0			[2]
NP	PN	phosphorus nitride	g	25.043	18.453	50.437	[5]
NS	SN	sulfur nitride	g	63.000	56.278	53.055	[5]
N <sub>2</sub>	N <sub>2</sub>	nitrogen	g	0	0	45.77	[1]
N <sub>2</sub> <sup>0</sup>	N <sub>2</sub> <sup>0</sup>	nitrous oxide	g	19.61	24.90	52.52	[1]
N <sub>2</sub> <sup>0</sup> <sub>3</sub>	N <sub>2</sub> <sup>0</sup> <sub>3</sub>	dinitrogen trioxide	g	20.01 12.02	33.32	74.61	[1] [1]
N <sub>2</sub> <sup>0</sup> <sub>4</sub>	N <sub>2</sub> <sup>0</sup> <sub>4</sub>	nitrogen tetroxide	g	12.19 -4.66	23.38 23.29	72.70 50.0	[1] [1]
N <sub>2</sub> <sup>0</sup> <sub>5</sub>	N <sub>2</sub> <sup>0</sup> <sub>5</sub>	nitrogen pentoxide	g c	2.7 -10.3	27.5 27.2	85.0 42.6	[1] [1]
N <sub>5</sub> P <sub>3</sub>	P <sub>3</sub> N <sub>5</sub>	phosphorus pentanitride	c	-71.4			[1]
O	O	oxygen monatomic	g	59.555	55.388	38.467	[1]
OP	PO	phosphorus monoxide	g	-1.455	-8.391	53.219	[3]
OS	SO	sulfur monoxide	g	1.5			[1]

Table I. Selected Thermodynamic Data (Cont.)

Empirical Formula	Functional Group Formula	Name	State	$\Delta H_f^{\circ}$ 298 kcal mole <sup>-1</sup>	$\Delta F_f^{\circ}$ 298 kcal mole <sup>-1</sup>	$S_f^{\circ}$ 298 cal mole <sup>-1</sup> deg <sup>-1</sup>	Ref.
O <sub>2</sub>	O <sub>2</sub>	oxygen diatomic	m=1 g aq	0 -2.8	0 3.9	48.996 26.5	[1] [1]
O <sub>2</sub> P	P <sub>2</sub> O	phosphorus dioxide	g	71.000	72.834	60.607	[7]
O <sub>2</sub> S	SO <sub>2</sub>	sulfur dioxide	g undissociated, m=1 100 H <sub>2</sub> O 200 H <sub>2</sub> O 500 H <sub>2</sub> O 1000 H <sub>2</sub> O 2000 H <sub>2</sub> O 5000 H <sub>2</sub> O 10000 H <sub>2</sub> O aq	-70.944 -76.6 -77.194 -78.054 -78.355 -78.811 -79.201 -79.642 -80.209 -80.584	-71.749 -71.872	59.30 38.7	[1] [1] [1] [1] [1] [1] [1] [1] [1]
O <sub>3</sub>	O <sub>3</sub>	ozone	g	34.1	39.0	57.08	[1]
O <sub>3</sub> S	SO <sub>3</sub>	sulfur trioxide	g c,β 105.41 -108.63	-94.21 -88.69 -88.04 -88.19	61.34 22.85 12.5	[1] [1] [1]	
O <sub>6</sub> P <sub>4</sub>	P <sub>4</sub> O <sub>6</sub>	phosphorus trioxide	c	-392.0			[1]
O <sub>10</sub> P <sub>4</sub>	P <sub>4</sub> O <sub>10</sub>	phosphorus pentoxide	c amorph -727	-713.2	-644.8	54.70	[1] [1]
P	P	phosphorus, monatomic phosphorus, white, α, c III phosphorus, red triclinic phosphorus, black phosphorus, red amorphous	g c c c amorph	0 -4.2 -9.4 -1.8	0 -2.9	38.978 9.82 5.45	[1] [1] [1] [1] [1]
PS		phosphorus sulfide	g	22.500	9.694	56.033	[5]
P <sub>2</sub>		phosphorus, diatomic	g	34.5			[1]
P <sub>2</sub> S <sub>3</sub>	P <sub>2</sub> S <sub>3</sub>	phosphorus trisulfide	c	-19.2			[1]
P <sub>4</sub>		phosphorus tetratomic	g	14.08	5.85	66.89	[1]
P <sub>4</sub> S <sub>3</sub>	P <sub>4</sub> S <sub>3</sub>	phosphorus sulfide	g c c	-19.408 -36.077 -37.000	-28.826 -37.513 -37.986	76.280 49.510 48.000	[3] [3] [3]
S	S	sulfur, rhombic sulfur, monoclinic sulfur monatomic	c c g	0 0.08 66.636	0 56.949	7.60 40.094	[1] [1] [1]
S <sub>2</sub>		sulfur diatomic	g	30.68			[1]
S <sub>3</sub>		sulfur triatomic	g	31.7			[1]
S <sub>4</sub>		sulfur tetratomic	g	32.7			[1]
S <sub>5</sub>		sulfur pentatomic	g	29.6			[1]
S <sub>6</sub>		sulfur hexatomic	g	24.5			[1]
S <sub>7</sub>		sulfur heptatomic	g	27.1			[1]
S <sub>8</sub>		sulfur octatomic	g	24.45	11.87	102.98	[1]

### References

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